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Cultură - Știință - Inovație din 1581



# Young Researchers' International Conference on Chemistry and Chemical Engineering (YRICCCE V)

May 8-10, 2025

Babeș-Bolyai University, Faculty of Chemistry and Chemical Engineering, Arany  
János 11, RO-400028, Cluj-Napoca

Sponsors:



simbolul calității

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## **YRICCCE V, Cluj-Napoca, May 8-10, 2025**

Dear colleagues,

We have the pleasure to welcome you in Cluj-Napoca to the fifth edition of the Young Researchers' International Conference on Chemistry and Chemical Engineering (YRICCCE V) which will be held in Cluj-Napoca, Romania, on May 8 - 10, 2025. We hope that this conference is a good opportunity for all participants to exchange ideas and experience in their own field of research and to open the way for future collaborations.

At the same time, we are seeking to offer you the opportunity to visit Cluj-Napoca, a city with a rich history and an important cultural center, as well as the privilege of visiting some unique landscapes and touristic attractions in the heart of Transylvania. We wish you fruitful participation in this scientific event and a pleasant stay in Cluj-Napoca.

The Organizing Committee

## Organizing Committee

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Institute of Food Science and Technology, Department of Nutrition

Prof. Dr. Livia Simon Sarkadi

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Prof. Dr. Péter Szalay

## Scientific Committee

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University of Szeged, Department of Inorganic and Analytical Chemistry

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Loránd Eötvös University, Institute of Chemistry

Prof. Dr. Péter Szalay



## Scientific Program

### Day 1 – Thursday, May 8<sup>th</sup>, 2025

Faculty of Chemistry and Chemical Engineering, Arany János 11

- 15:00 – 17:00**      **Registration**
- 17:00 – 17:15**      **Opening**
- 17:15 – 17:45**      **Plenary lecture 1**, chaired by Prof. Livia Simon Sarkadi /  
Prof. Katalin Várnagy

**Dr. habil. Elisabeta I. Szerb**, Senior Researcher, CS I  
*"Coriolan Dragulescu" Institute of Chemistry, Timișoara, Romania*  
**Electrochemical sensors based on ordered “soft” hybrid materials**

- 18:00 – 21:00**      **Welcome Party**

### Day 2 – Friday, May 9<sup>th</sup>, 2025

Faculty of Chemistry and Chemical Engineering, Arany János 11

- 09:00 – 09:30**      **Plenary lecture 2**, chaired by Prof. Anca Silvestru

**Dr. habil. József Kupai**, Associate professor  
*BME Faculty of Chemical Technology and Biotechnology, Department  
of Organic Chemistry and Technology, Budapest, Hungary*  
**Sustainable application and recycling of organocatalysts**

- 09:30 – 12:45**      **Oral presentations**

**1<sup>st</sup> Session** chaired by Dr. habil. Elisabeta I. Szerb

- 09:30 – 09:45**      **O1.** Marțian Paul Cristian  
*Novel Cationic Covalent Organic Framework applied for Chloramphenicol  
detection*
- 09:45 – 10:00**      **O2.** Cătălina Diana Ușurelu  
*A study on the modification of nanocellulose with a naturally occurring aldehyde  
possessing antibacterial properties*
- 10:00 – 10:15**      **O3.** Mihály Mátyás Rudolf

## YRICCCE V, Cluj-Napoca, May 8-10, 2025

### *Processes Behind the Enhanced Luminescent Chromium-Doped Zinc Gallate Nanocrystals*

10:15 – 10:30 O4. Ana Varadi

*ZnO nanostructures with different morphologies for supercapacitor applications*

**10:30 – 11:00 Coffee break**

### **2<sup>nd</sup> Session** chaired by Dr. Adrian-A. Someșan

11:00 – 11:15 O5. Rahaf Akel

*Half-sandwich Type Platinum-group Metal Complexes of Isoxazol(in)e Glycoconjugates: Synthesis and Evaluation as Anticancer and Antimicrobial Agents*

11:15 – 11:30 O6. Ioan Stroia

*Artificial anion transmembrane transporters: from nitrate-selective to efficient chloride electrogenic and electroneutral transport*

11:30 – 11:45 O7. Bertalan Varga

*Electrostatic Immobilization of Cyclodextrins Containing Permanent Positive Charges – Wastewater Monitoring in Focus*

11:45 – 12:00 O8. Alex Florin Isai

*Boronic acids with self-assembling properties as potential candidates for artificial water channels*

12:00 – 12:15 O9. Alshimaa I. Zaki

*New Half-Sandwich Platinum-Group Metal Complexes with Hetaryl-Substituted N- and C-Glucopyranosyl-1,2,3-Triazole Chelators: Synthesis, Anticancer, and Antimicrobial Potential*

12:15 – 12:30 O10. Aiman Aitkazina

*Synthesis and Characterization of Polymer Conetworks from Sulfur-Containing Copolymers*

12:30 – 12:45 Dr. Albert Soran CCDC

*The CSD ecosystem - an overview of benefits from structural science.*

**13:00 – 15:00 Lunch break**

**15:00 – 16:45 Oral presentations**

### **3<sup>rd</sup> Session** chaired by Dr. Albert Soran

15:00 – 15:15 O11. Valeria Danilova

*Application of new chelating resin in brine hardness removal to feed the chlor-alkali membrane cell process. I. Optimization using response surface methodology*

15:15 – 15:30 O12. Andrea Bogyor

*Clorhexidine digluconate adsorption studies*

- 15:30 – 15:45      O13. Niloofar Bayat  
*Thermal Decomposition Pathways of Hexaamminecobalt (III) Dibromide Permanganate: Insights into Cobalt-Manganese Oxide Spinel Formation and Photocatalytic Intermediates*
- 15:45 – 16:00      O14. Cătălin Eduard Șalgău  
*Heteroleptic diorganoselenides based on pyridine and pyrazole functionalities. Synthesis, structural characterization and coordination behaviour*
- 16:00 – 16:15      O15. Robert Botea  
*Rational Design and Synthesis of Zn(II) Complexes with Polydentate Schiff Base Ligands*
- 16:15 – 16:30      O16. Raffaele Fontana  
*Study on the reactivity of organobismuth(I) compounds towards ortho-quinones*
- 16:30 – 16:45      O17. Marcell Tátrai  
*Morphological features dictate drug release from nanostructured borosilicate – alginate aerogels and xerogels*

**16:45 – 17:30      Poster session + coffee break**

- P1. Larisa Silveșan  
*Monitoring reaction kinetics in the determination of antioxidant activities of phenolic compounds*
- P2. Sânziana-Maria Varodi  
*Encapsulation of anthocyanins from Vaccinium vitis-idaea extracts*
- P3. Sergiu-Raul Cosma  
*No Heme-Chlorite Adduct in the Catalytic Cycle of Chlorite Dismutase: Insights From QM/MM and Dynamics Calculations*
- P4. Alexandru Paul Rus  
*New analytical methods for quantification of Hg species in soft water using HPLC-ICP-MS technique*
- P5. Ana-Ioana Paris  
*LC-MS/MS method for the determination of perfluoroalkyl sulfonic acids in dehydrated sludge from wastewater treatment plants*
- P6. Eunice Fatoye  
*POLYACRYLIC ACID GEL-BASED ELECTROLYTES FOR RECHARGABLE Zn-AIR BATTERIES*
- P7. Aron Rop



*Rapid synthesis of Thermoresponsive PNIPA-b-PNAM Block Copolymers*

P8. Veronika Csilla Pardi-Tóth

*Synthesis and study of multiblock copolymers of acrylamide derivatives*

P9. Nicoleta Sandu

*Design and synthesis of poly-functionalized azides for “click” chemistry-based microscopy applications*

P10. Levente Biró

*Synthesis of New Coumarin Derivatives*

P11. Mihai-Alexandru Molența

*1,3,4-Oxadiazole core as building block for fluorescent materials design*

P12. Mihaela Tudorache

*Assessment of the Antifungal Activity of Grape Pomace Extracts*

P13. George Daniel Tudorache

*The Prediction Performance of Statistical Models and Neural Networks in a Microgrid Based on Energy Consumption from Renewable Sources*

P14. Eleonóra Kapronczai

*Synthesis, Structure and Reactivity of a New Pyrazole-Containing Homoleptic Diorganotellurium(II) Compound*

P15. Narcis-Teodor Niță

*Biocomposite materials based on sawdust biomass and natural polymers: Synthesis, characterization and potential for biosorption applications*

P16. Tudor Marius Ungurean

*Synthesis and characterization of novel azastibocine halides*

P17. Bradut Bogdan Minea

*Pesticide and heavy metals residues in citrus fruits: human exposure and risks*

**17:30 – 19:00      Oral presentations**

**4<sup>th</sup> Session** chaired by Dr. Niculina Hădade

17:30 – 17:45      O18. Diana-Oana Rusu

*Photophysical studies on thin films of hybrid liquid crystalline materials based on an emissive metallomesogen*

17:45 – 18:00      O19. Máté Benedek

*Synthesis and electrochemical testing of polyacrylic acid based hydrogel electrolyte for Zn–air battery*

18:00 – 18:15      O20. Bence András Sármézey

## YRICCCE V, Cluj-Napoca, May 8-10, 2025

*Thermoresponsive LCST-type Random Copolymers with PEG Methyl Ether Methacrylate of 1100 g/mol Molecular Weight: The Effect of Composition and the CST of the Homopolymers*

18:15 – 18:30 O21. Ana Varadi

*Defects Induced by Lithium in ZnO Nanorods Used for Supercapacitor Applications*

## Day 3 – Saturday, May 10<sup>th</sup>, 2025

Hotel Universitas, Pandurilor 7

**09:30 – 11:00 Oral presentations**

**5<sup>th</sup> Session** chaired by Dr. Alexandra Pop

09:30 – 09:45 Dr. Lavinia Buta MDPI

*The World of Open Access and Ethics in Publishing*

09:45 – 10:00 O22. Gabriela-Mădălina Oprică

*The modification of nanocellulose with a sulfated polysaccharide: A physico-chemical study*

10:00 – 10:15 O23. Gomaa Elsayed Amer

*Coordination Chemistry Behaviour of Cu(II), Zn(II) and Ni(II) with Some Native and Phosphorylated Tau Protein Peptides*

10:15 – 10:30 O24. Adrian Brânzanic

*Intraprotein Electron Routes in Ascorbate/Caffeate - Myoglobin Systems*

10:30 – 10:45 O25. Melinda Tamas

*Structural aspects in organotin(IV) selenolates*

10:45 – 11:00 O26. Darius Dumitraş

*Synthesis, structural characterization and reactivity of new pyridine based organoselenium compounds*

11:00 – 11:15 O27. Faareha Mazhar

*Metal binding ability of tau (289-300) fragment*

11:15 – 11:30 O28. Alexandru Vişan

*Hybrid supramolecular ordered materials based on metallomesogens for electrochemical sensing*

**11:30 – 12:00 Closing remarks**

**PLENARY LECTURES**

**PL1 – PL2**

## Electrochemical Sensors Based on Ordered “soft” Hybrid Materials

Elisabeta I. Szerb

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Electrochemical sensors are promising tools for the detection of analytes in biomedicine, food science and environmental science due to their highly sensitive and selective detection, rapid response, easy operation and miniaturization [1]. Due to the progress in these application fields, a proper electroactive material is required to be highly efficient, performing multiple functions, to be of low cost and so on, conditions that can be fulfilled by hybrid materials, obtained by mixing several precursors, each able to perform a certain function. While increasing the number of precursors forming the sensing material, their properties are not just the sum of the component's properties, but new and synergistic ones derive by close contact or mutual spatial arrangements of the molecules or nanoparticles, improving the sensitivity or selectivity. However, controlling the nanostructuring and morphology of the final sensing material, essential for its reproducibility, becomes more difficult as the nature of the components differ or their number increases. One of the most important aspects is to relate the nature, structure and supramolecular arrangements of the components to explain the mechanism of action and to obtain data for a further design of materials with optimized sensing properties.

Thus, the procedure of immobilization or modification of the electrode surface is a complex and a delicate key step in repeatability and reproducibility of electrode fabrication. Developing hybrid electrode materials with controlled supramolecular order is highly desirable in theory and practice. Nanostructured carbon-based electrodes modified with metal-based nanomaterials bring together the electrical, optical, thermal properties, mechanical stability and electrical conductivity of carbons with excellent physicochemical properties of metals [2]. Taking advantage of the ability to be spread uniformly forming self-healing ordered films when in the mesophase, metallomesogens mixed with nanosized carbons may generate nanostructured liquid crystalline hybrid materials with well determined and controlled order and distribution of components, hence ordered metal oxide electroactive centers following electrochemical (EC) reduction.

On this background the recent progress in the design and applications of electrochemical sensors will be presented, highlighting the results obtained by the use of ordered nanostructured hybrid paste electrodes for the detection of bioanalytes or emerging pollutants [3].

*Acknowledgements:* This work is supported by Romanian Academy, Program 4.

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## Sustainable Application and Recycling of Organocatalysts

József Kupai

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In 2021, Benjamin List and David W. C. MacMillan were awarded the Nobel Prize in Chemistry for their discovery of asymmetric organocatalysis, which underscores the significance of chiral organocatalysts in stereoselective synthesis [1].

Cinchona alkaloid derivatives are highly valued due to their versatility and the ability to fine-tune asymmetric reactions [2–4]. Recycling these catalysts is crucial for sustainability, and we have explored various methods for this, including the attachment of these alkaloids to solid supports [2], membrane separation [3], and solvent exchange [4].

Bifunctional hydrogen-bonding organocatalysts, such as cinchona thioureas and cinchona squaramides, are essential in catalysis because they activate and orient substrates through hydrogen bonding [3, 4]. Our research has led to the development of cinchona alkaloid-based organocatalysts for stereoselective reactions, including (aza)-Michael [3–5] and aza-Diels-Alder [5] reactions, which produce pharmaceutical intermediates. Additionally, we have found that substituting carbonyl groups with thiocarbonyl groups in squaramide-type catalysts increases their acidity, facilitating new catalytic reactions [5].

We have also concentrated on utilizing organocatalysts for sustainable plastic recycling, specifically in the depolymerization of PET [6] and BPA-PC [7] into reusable monomers. Furthermore, we have developed a novel bio-based solvent, MeSesamol, which provides a greener alternative for chemical processes, supporting sustainable catalysis and plastic depolymerization [8].

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**ORAL PRESENTATIONS**  
**O1 – O28**

## **Q1 Novel Cationic Covalent Organic Framework Applied for Chloramphenicol Detection**

Paul-Cristian Martian<sup>1</sup>, Mihaela Tertis<sup>1</sup>, Catalin-Constantin Anghel<sup>2</sup>, Daniel-Florin Bogosel<sup>2</sup>, Dan-Alexandru Toc<sup>3</sup>, Carmen Costache<sup>3</sup>, Lucian Barbu-Tudoran<sup>4</sup>, Niculina-Daniela Hadade<sup>2</sup>, Cecilia Cristea<sup>1</sup>

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**Introduction:** Covalent organic frameworks (cCOFs) are crystalline porous polymers well known for their permanent porosity and ordered structures, making them suitable for biomedical applications [1]. Chloramphenicol (CAP) is an efficient broad-spectrum antibiotic that inhibits bacterial protein synthesis, though its use is limited by serious side effects. This study presents an electrochemical method for detecting CAP in pharmaceutical formulations using carbon screen-printed electrodes (C-SPE) combined with COFs to improve sensitivity and specificity.

**Material and Methods:** cCOF I (Figure 1) with imine connections was synthesized through the reaction between 2-((5-(trimethylammonium)pentyl)oxy)benzene-1,4-diammonium hydrochloride and benzene-1,3,5-tricarboxaldehyde, under solvothermal conditions. C-SPE electrodes were modified with an aqueous suspension of chitosan and cCOF I. CAP was preconcentrated on the modified surface and detected using cyclic voltammetry (CV) in a Britton-Robinson buffer at pH 6. The detection method was applied to CAP in various pharmaceutical products. The antimicrobial activity of cCOF I was assessed against 7 pathogenic bacteria.

**Results:** The developed sensor demonstrated a broad detection range, low limit of detection, high specificity, and effective results in electrochemical detection of CAP.

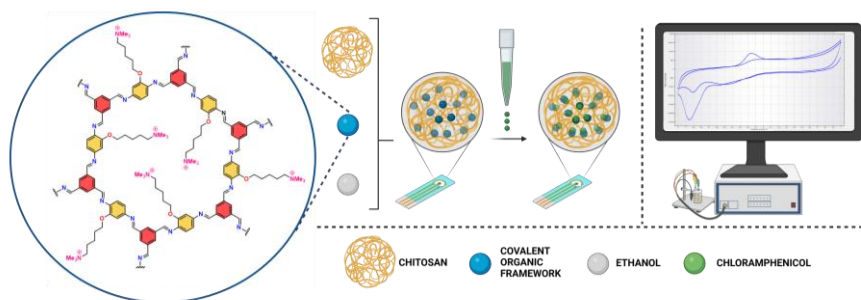


Figure 1: The detection of CAP through CV procedure utilizing cCOF I.

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## **O2 A Study on the Modification of Nanocellulose with a Naturally Occurring Aldehyde Possessing Antibacterial Properties**

Cătălina-Diana Uşurelu<sup>1,2</sup>, Gabriela Mădălina Oprică<sup>1,2</sup>, Cristina Firincă<sup>1</sup>, Cristian Andi Nicolae<sup>1</sup>, Adriana Nicoleta Frone<sup>1</sup>, Mircea Teodorescu<sup>2</sup>, Denis Mihaela Panaitescu<sup>1</sup>

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Natural materials constitute a valuable source for the development of innovative products. One of the most remarkable green nanomaterials is nanocellulose (NC), which is obtained from abundant and inexhaustive cellulose resources and waste [1]. The list of NC's properties useful for different applications is large and includes, among others, a high specific surface area, biodegradability, biocompatibility, high-water uptake, excellent mechanical strength, good chemical resistance, as well as plenty of possibilities for chemical modification [2]. Unfortunately, NC does not possess antibacterial properties, which are mandatory for biomedical and packaging applications [3].

In this work, a naturally occurring aldehyde extracted from cinnamon, with recognized activity against bacteria, was used to induce antibacterial properties to NC and modify its hydrophilic-hydrophobic balance in a controlled manner. Different physical and chemical approaches were used to incorporate the natural aldehyde in NC and its effect on the structure, morphology, thermal, and antibacterial properties of NC were assessed. Fourier-transform infrared spectroscopy, Raman spectroscopy, scanning electron microscopy, thermogravimetric analysis, and contact angle measurements provided information about the properties of the new biomaterials.

Modifying NC with the cinnamon-derived aldehyde represents a green, inexpensive, and facile route for inducing antibacterial activity to NC and for adjusting its hydrophilic-hydrophobic balance.

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### **O3 Processes Behind the Enhanced Luminescent Chromium-Doped Zinc Gallate Nanocrystals**

Mátyás M. Rudolf<sup>1,2</sup>, Gábor Bortel<sup>2</sup>, Bence G. Márkus<sup>3</sup>, Ádám Gali<sup>2</sup>, David Beke<sup>2,3</sup>

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Zinc gallate nanocrystals with dopants have wide applications due to their optical properties that can be engineered by using different methods for synthesis, selecting co-dopants, or adding various semiconductors to the system. In our works we have successfully improved the near-infrared emission of the chromium-doped zinc gallate (ZGO:Cr or ZGC) nanocrystals with a magnitude under X-ray irradiation. With these enhancements, this material is getting closer to be a promising nanoprobe for background-free deep-tissue bioimaging or an activator for photodynamic- or photon-induced therapy (PDT/PIT).

We have added ultrasmall, 1-3 nm sized SiC nanoparticles to create core-shell nanoparticles (ZGC-SiC) with enlarged emission around 700 nm. Besides the background of the improved optical properties, we have studied the role of the SiC nanoparticles in the nucleation process during the hydrothermal reaction with several measurements [1]. We have also analyzed the effect of the post-annealing process using treatments with different temperatures on the hydrothermally synthesized nanocrystals. Annealing treatments were done on the samples with and without added silica to avoid further crystal growth. We have also studied the long-lasting luminescent (LLP) behaviours of the samples under X-ray and UV- excitations. We have estimated the treatment time for therapy from the integration of the overlap between the absorption spectra of an anticancer agent drug (IR700-mAb) and the emission spectra of our brightest sample [2].

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## **O4 ZnO Nanostructures with Different Morphologies for Supercapacitor Applications**

Ana Varadi<sup>1,2</sup>, Dana Toloman<sup>2</sup>, Maria Stefan<sup>2</sup>, Adriana Popa<sup>2</sup>, Arpad Rostas<sup>2</sup>, Sergiu Macavei<sup>2</sup>, Cristian Leostean<sup>2</sup>, Emre Erdem<sup>3</sup>

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Supercapacitors (SCs) are energy storage devices that play a major role in matching the upcoming energy demand [1]. Compared to the popular energy storage devices, SCs have a high power density as opposed to batteries and high energy density as opposed to capacitors, bridging the gap between them [2]. A SC consists of four major components: electrodes, electrolytes, separators and collectors, and among these the electrode material is the most tailored to improve the SC's performance [3]. In this study ZnO with different morphologies was studied as electrode material for SC devices. Thus, morphology-dependent ZnO nanoparticles were prepared using several methods: hydrothermal (nanorods), solvothermal (nano-pyramids, nano-hexagons, and nanobullets), and chemical precipitation (nano-flowers). All materials were thoroughly characterized by scanning/transmission electron microscopy, X-ray diffraction, and spectroscopic techniques like photoluminescence, UV-vis, Raman, and electron paramagnetic resonance spectroscopy. Subsequently, the ZnO-based materials were assembled in symmetric supercapacitor devices to test their energy storage capabilities. The ZnO with nanorod and hexagonal morphologies showed the best specific capacity (180 and 142 F/g), energy density (25 and 19 Wh/kg), and power density (211 and 252 kW/kg) values. The defect centers in materials play a crucial role in ZnO materials' energy storage capacity.

*Acknowledgements:* This work was supported through the Ministry of Research, Innovation and Digitalization, Romania's National Recovery and Resilience Plan, PNRR-III-C9-2022-I8, CF 163/15.11.22, financing contract no. 760097/23.05.23.

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## **O5 Half-sandwich Type Platinum-group Metal Complexes of Isoxazol(in)e Glycoconjugates: Synthesis and Evaluation as Anticancer and Antimicrobial Agents**

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Due to the toxicity and the development of platinum resistance over time of platinum-based chemotherapeutics such as cisplatin, oxaliplatin, and carboplatin, extensive research is being conducted to develop new compounds that could provide greater therapeutic benefits [1][2].

In our previous publications, we provided a detailed description of the synthesis of half-sandwich type complexes involving platinum-group metal ions (Ru(II), Os(II), Rh(III), and Ir(III)) with O-protected C- and N-glycosyl heterocyclic N,N-bidentate ligands (pyridin-2-yl or quinolin-2-yl substituted 1,2,4- and 1,3,4-oxadiazoles, and 1,2,3-triazoles). These complexes demonstrated promising anticancer and antimicrobial effects, which were found to be strongly correlated with the tested azole moieties [2][3]. In this work our aim was to investigate the effect of a new heterocycle, namely isoxazol(in)e coupled to various sugar forms on the biological efficiency.

We synthesized a library of half-sandwich complexes with N,N-bidentate monosaccharide ligands.

Per-O-acetylated or benzoylated glycoconjugates of isoxazoline were prepared in cycloaddition reactions, while several reaction conditions were tested to prepare the per-O-benzoylated glycoconjugates of isoxazoles. O-Benzyl protected glycoconjugates were prepared in a cycloaddition reaction followed by a one-step protecting group exchange from benzyl to benzoyl.

Half-sandwich type metal complexes with bidentate O-unprotected monosaccharide ligands were also prepared to investigate the effect of protecting groups on the biological activity. The distribution coefficient of the synthesized complexes (logD) was determined. Further details of the syntheses and biological activity of the new compounds will be presented in the conference.

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## O6 Artificial Anion Transmembrane Transporters: from Nitrate-Selective to Efficient Chloride Electrogenic and Electroneutral Transport

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The artificial transmembrane transport of anions, particularly chloride, has emerged as an innovative approach to address two significant medical challenges: *i*) replacing defective natural channels to treat diseases associated with channelopathies, such as cystic fibrosis [1], and *ii*) inducing cancer cell death through apoptosis or autophagy disruption pathways in malign cells [2]. Herein we disclose three series of molecular clefts (Figure 1) finely tailored to *i*) clarify the impact of hydrogen bonding donor strength (CH vs NH vs NH&OH donors) on transport selectivity and *ii*) target specific applications, namely channel replacement therapy with chloride uniporters (NH and some NH&OH donors) and induced cancer cell death with chloride/proton cotransporters. We also performed DFT and MD simulations to gain useful insights on transmembrane transport mechanisms.

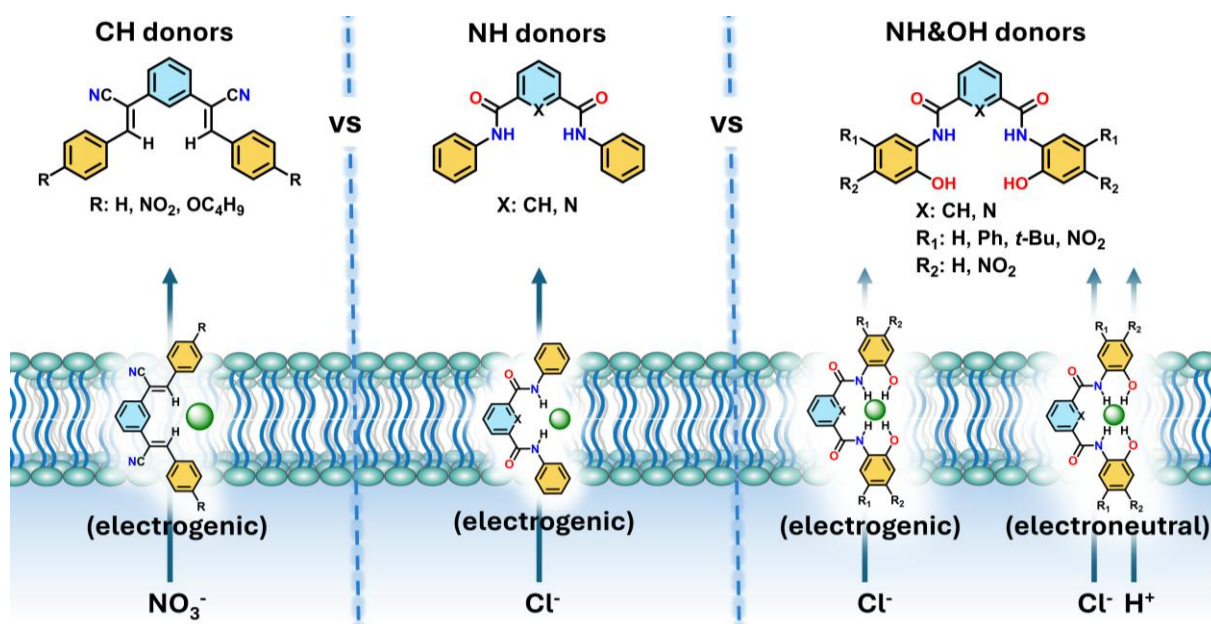


Figure 1: The structures of CH donor clefts mediating preferentially NO<sub>3</sub><sup>-</sup> uniport (left), NH donors mediating Cl<sup>-</sup> uniport (middle) and NH&OH clefts mediating both Cl<sup>-</sup> uniport as well as Cl<sup>-</sup>/H<sup>+</sup> symport.

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## **O7 Electrostatic Immobilization of Cyclodextrins Containing Permanent Positive Charges – Wastewater Monitoring in Focus**

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Cyclodextrins (CDs) are macrocycles composed of  $\alpha$ -D-glucopyranose units. These macrocycles are known about their excellent complexing ability. Due to their polar surface and apolar cavity, CDs are able to form inclusion complexes with APIs, solvents or even with CO<sub>2</sub> [1]. They are soluble in water and can therefore be used to improve the solubility or shelf-life of organic substances [2]. In addition to solubilization, CDs can also be used to remove water pollutants [3].

The aim of our research is to synthesize positively charged CD derivatives, which can be immobilized on various solid phases (e.g. silica gel, cation exchange resin) via electrostatic interaction for the development of new SPE (solid phase extraction) packings. Petr *et al.* have already proved the suitability of this method by anchoring several beta cyclodextrin (BCD) derivatives on an anionic membrane for the separation of tryptophan enantiomers [4]. During our research work, a set of known and novel BCD derivatives were prepared containing permanent positive charges. Their immobilization was performed on sulfonylpropyl-modified silica gel with different particle sizes. The synthesized CDs could effectively complex APIs (acetylsalicylic acid, diclofenac, ibuprofen), hormones (17- $\beta$ -estradiol, estrone) and other endocrine disruptor chemicals (EDCs, e.g. bisphenol A and 4-nonylphenol), which remain in the wastewater after the currently used purification treatments. Our results demonstrate the applicability of this kind of SPE packings for wastewater analysis, however, the type of solid support and the structure of the CDs need to be optimized. Our future goal is the preparation of reusable SPE cartridges that are more efficient and selective than the reversed phase cartridges available on the market.

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## O8 Boronic Acids With Self-Assembling Properties as Potential Candidates for Artificial Water Channels

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Boronic acids are a class of organic compounds known for their structural versatility that have found applications as valuable intermediates in organic synthesis [1]. Additionally, they are important players in diverse biomedical applications, including sensor design and drug production [2]. Their ability to selectively interact with vicinal hydroxyl groups has been used to facilitate the transport of monosaccharides through liquid organic membranes [3]. Given their excellent capacity for selective molecular recognition and transport, along with the growing interest of researchers in selective water transport [4], boronic acids have emerged as promising candidates for designing artificial water channels (AWCs).

Our work focused on the synthesis, structural characterization, and investigation of the transport properties of a series of new phenylboronic acids functionalized with alkylurea units (Figure 1). Their structures were confirmed by <sup>1</sup>H-NMR, <sup>13</sup>C-NMR, and HRMS (APCI+). Water transport ability was assessed through stopped-flow light scattering experiments. Preliminary tests yielded highly promising results, suggesting that these compounds are noteworthy candidates for the development of new artificial water channels.

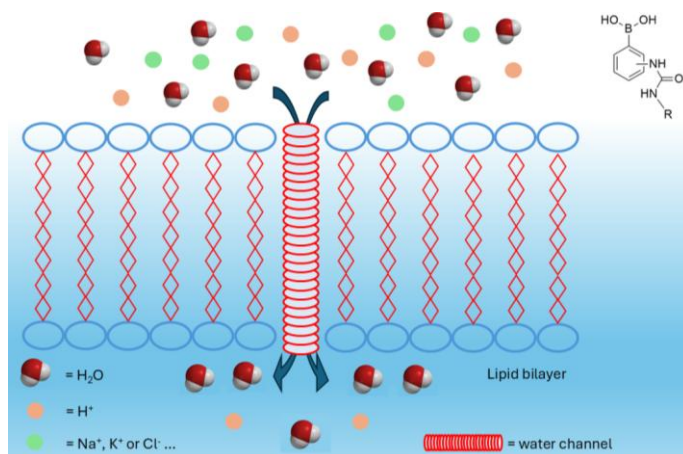


Figure 1: The general structure of the target compounds and the schematic representation of an artificial water channel and its operating mechanism.

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## O9 New Half-Sandwich Platinum-Group Metal Complexes with Hetaryl-Substituted *N*- and *C*-Glucopyranosyl-1,2,3-Triazole Chelators: Synthesis, Anticancer, and Antimicrobial Potential

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Platinum (II) complexes like cisplatin, oxaliplatin, and carboplatin are widely used; however, their poor selectivity and diminishing efficacy over time necessitate new therapeutic alternatives [1]. Recent research has focused on Ru(II), Os(II), Ir(III), and Rh(III) complexes. Our research group have synthesized a series of such complexes incorporating *N*- and *C*-glucopyranosyl azole-based *N,N*-bidentate ligands (**Fig. 1, I**). A variety of them demonstrated (sub)micromolar cytostatic activity against different cancer cells and exhibited bacteriostatic effects against multidrug-resistant Gram-positive bacteria [2]. Complex (**II**) proved to be the most potent member of the series. As a continuation of this project, further modifications were carried out including changes in anomeric configuration from  $\beta$  to  $\alpha$  (**III-A**) and heterocycle conjugation mode to *C*-glycosylic analogs (**III-B**). The synthesis as well as the anticancer and antimicrobial evaluation of these newly developed sugar-based heterocyclic ligands and their metal complexes, will be detailed in the oral presentation.

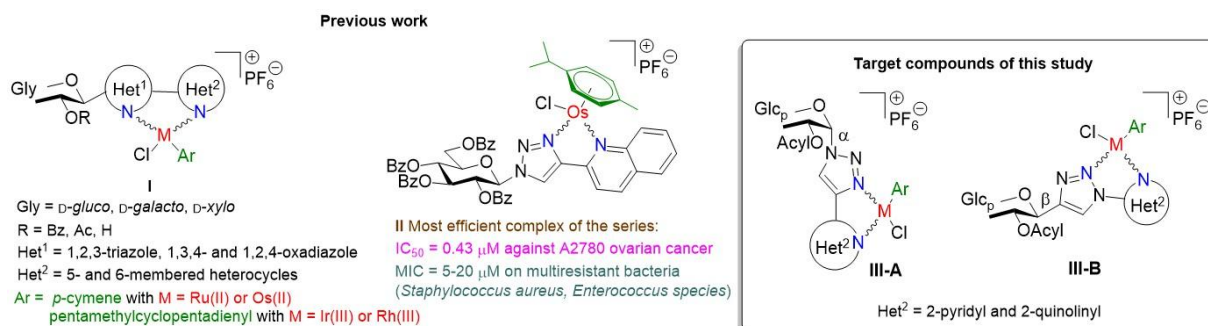


Figure 1. Highlights of our previous study and target compounds of this work.

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## **O10 Synthesis and Characterization of Polymer Conetworks from Sulfur-Containing Copolymers**

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Sulfur-containing polymers have gained increasing attention due to their unique properties and potential applications. Among various synthesis methods, the thiol-ene Michael addition offers an efficient route for incorporating sulfur into polymer structures. In this study, a novel approach was developed to simultaneously perform thiol-ene Michael addition and oxidative thiol coupling, yielding a copolymer of 3,6-dioxaoctanedithiol and poly(ethylene glycol) diacrylate (P(DODT-co-PEGDA)) with thioether and disulfide groups.

The synthesized copolymer can be used as macrocrosslinker to form polymer conetworks via copolymerization with methyl acrylate (MA) (see a photo in Figure 1 on a resulting conetwork). Reduction studies revealed that breaking disulfide bonds significantly altered the conetwork properties, leading to structural disintegration.

These novel polymer networks are expected to have advantageous properties which can be harnessed in catalysis and drug delivery.



*Figure 1: A photo on a poly(methyl acrylate)-*l*-P(DODT-co-PEGDA) conetwork*



## **O11 Application of New Chelating Resin in Brine Hardness Removal to Feed the Chlor-Alkali Membrane Cell Process.**

### **I. Optimization Using Response Surface Methodology**

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Membrane cell chlor-alkali processes produce chlorine ( $\text{Cl}_2$ ), hydrogen ( $\text{H}_2$ ) and sodium hydroxide ( $\text{NaOH}$ ) by electrolysis of a nearly saturated salt solution. The higher current densities of the present technology (membranes zero-gape) have increased the demand for higher brine purity to ensure electrolysis efficient performance by minimal energy consumption [1]. Using the ultrapure brine in membrane electrolytic cells improves current efficiency and reduces the damage caused by harmful metal ions from initial brine [1, 2]. The brine hardness content is lowered from 3 to 5 ppm to less than 20 ppb (ultrapure brine conditions) by ion exchange using polymer resins that must have a good exchange capacity and a special affinity for retaining of  $\text{Ca}^{2+}$  and  $\text{Mg}^{2+}$  ions. These materials' data sheets from the producers inform about the total ion exchange capacity for the resin delivery form [3]. The literature lacks sufficient experimental research that scientifically explains the behaviour and the performance of the new commercial resins and also investigations on the kinetics and thermodynamics of the brine hardness purification process.

The practical ion exchange capacity of *Lewatit® MonoPlus TP 208* resin (by Lanxess [3]) for  $\text{Ca}^{2+}$  and  $\text{Mg}^{2+}$  ions removal was investigated. In the experiments both industrial brine (by Chimcomplex Borzesti RO) and binary synthetic solutions containing  $\text{Ca}^{2+}$  and  $\text{Mg}^{2+}$  ions respectively were used. Preliminary batch ion-exchange experiments were conducted to determine the effect of resin dose, pH of the solution, initial brine hardness concentration, temperature, contact time solid – liquid. For the main phase of experiments, batch ion-exchange tests were conducted based on a  $3^2$  factorial design with pH, temperature and initial hardness concentration in the solution as the independent variables. Factorial design and response surface methodology were applied to evaluate and optimize the effects of specific conditions of ion-exchange process. This preliminary study allows for the subsequent implementation of the ion-exchange brine purification process in dynamic mode. The final objective of the study is the transposition to an industrial scale, so that the secondary brine purification process can be exploited industrially in optimal conditions with maximum efficiency.

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## **O12 Chlorhexidine Digluconate Adsorption Studies**

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Chlorhexidine digluconate (CHD) is a widely employed biocide in various products designed for either human, or animal use. As such, it is usually discharged in municipal sewages, and since it is not biodegradable, it poses a threat to the bacterial colonies in wastewater treatment facilities. If it is discharged directly into the environment, it might accumulate [1], and hence affect aquatic life, even at concentrations as low as 45 µg/L [2].

Adsorption is one of the most effective ways of removing toxic species from water [3,4], with paper being an environmentally friendly and renewable adsorbent source [3,4]. Hence this work aimed to establish the kinetic, mechanistic, and thermodynamic aspects of CHD adsorption on commercially available household paper.

Batch experiments were carried out by using synthetic CHD aqueous solutions with variable  $m_{0,CHD}/m_{paper}$  mass ratios and at different temperatures. The advance of the process was monitored spectrophotometrically at 231 nm. The kinetics of the overall process proved to be of pseudo-second order and controlled by the diffusion within the paper's pores. Equilibrium data were best in agreement with the Langmuir isotherm.

*Acknowledgements:* The authors acknowledge TEAM ANDAVA (Voluntari, Romania) for kindly providing the ANA Chlorhexidine 2% Aqueous Solution used in experiments, as well as Dr. Alina Filip from the Babeş-Bolyai University for her kind help in the microbiology tests.

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# O13 Thermal Decomposition of Hexaammine Cobalt(III) Dibromide Permanganate: From Spinel Formation to Photocatalytically Active Intermediates

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The thermal decomposition of hexaamminecobalt(III) dibromide permanganate was studied as a precursor for Co–Mn composites. The process produced  $\text{Co}_{1.5}\text{Mn}_{1.5}\text{O}_4$  spinel under air, while inert conditions resulted in different crystalline phases confirmed by several characterization techniques such as TG-MS, XRD, IR, SEM-EDX. The intermediates formed at 300°C and 500°C exhibited distinct phases, including hydrated cobalt(II) bromide and cobalt(II) oxide. These products showed promising photocatalytic activity in the degradation of Congo Red dye under UV light, with enhanced degradation rates observed at pH 5.2 compared to pH 3.6. The intermediates demonstrated up to 22 times faster degradation rates, highlighting their catalytic potential.

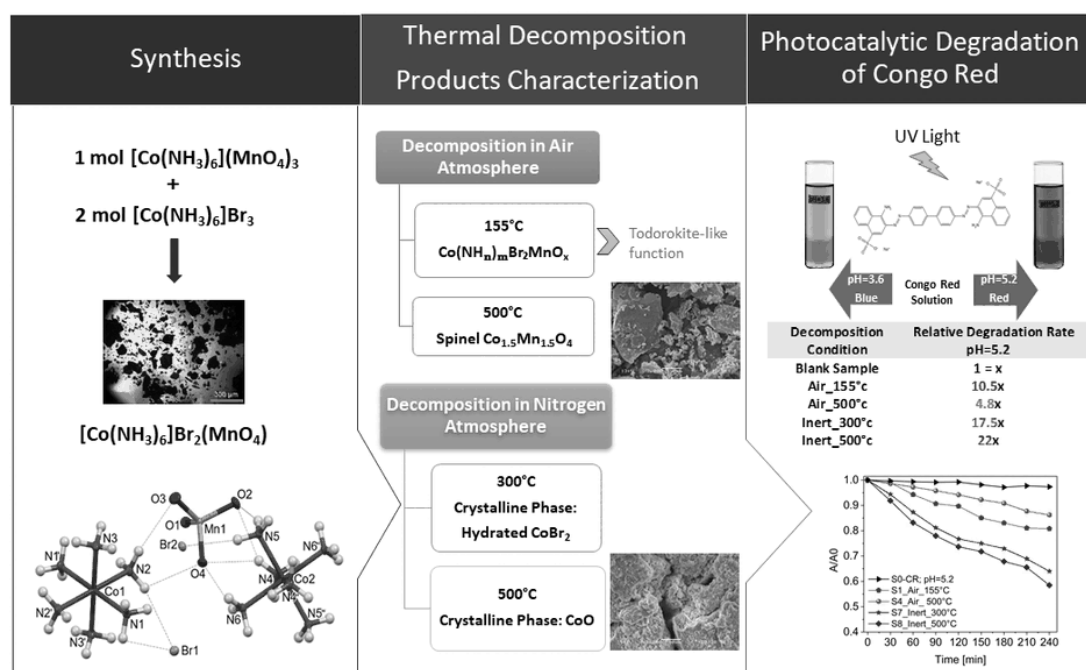


Figure 1: Graphical abstract

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## **O14 Heteroleptic Diorganoselenides Based on Pyridine and Pyrazole Functionalities. Synthesis, Structural Characterization and Coordination Behaviour**

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In the last years, nitrogen containing heterocycles have proven to be valuable components in synthesis of novel biological or catalytic active species owing to the hard Lewis base character of the donor atom that is essential in the design of good ligands suitable for synthesis of metal complexes with potential applications in various fields such as organic synthesis or medicine [1-5].

Following recent developments in synthesis of derivatives based on pyridine and pyrazole, in this work diorganoselenides 2-[(pyridin-2-ylmethyl)selenyl]pyridine (**L1**) and 2-[(2-(1*H*-pyrazol-1-yl)ethyl)selenyl]pyridine (**L2**) have been synthesized starting from 2,2'-dipyridyl diselenide and have been used in complexation reactions with silver(I) salts to obtain six new complexes containing AgOTf, AgNO<sub>3</sub> or AgPF<sub>6</sub>.

The compounds have been structurally characterized in solution by multinuclear NMR Spectroscopy (<sup>1</sup>H, <sup>13</sup>C, <sup>19</sup>F, <sup>31</sup>P, <sup>77</sup>Se, as appropriate) and mass spectrometry. The crystal and molecular structures of the silver(I) complexes [(**L1**)Ag]OTf (**1**), [(**L1**)Ag]NO<sub>3</sub> (**2**), [(**L2**)Ag]OTf (**4**) and [(**L2**)Ag]PF<sub>6</sub> (**6**) were determined by single crystal X-ray diffraction.

In solid state, both ligands act as bimetallic triconnective bridging moiety with 1κN:2κ<sup>2</sup>N,Se connectivity leading to the formation of dimeric or polymeric units. In solution, conductivity measurements suggest a 1:1 electrolytes behaviour in MeOH solutions of the compounds **1-6**. In the crystal structure of compound **6**, a supported argentophilic interaction is established with a Ag1...Ag1' distance of 2.9302(6) Å.

*Acknowledgements:* Financial support from UEFISCDI (PN-IV-P1-PCE-2023-0966) is highly acknowledged.

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## **O15 Rational Design and Synthesis of Zn(II) Complexes with Polydentate Schiff Base Ligands**

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The development of polydentate imino and amino ligands has significantly advanced the design of Zn(II) coordination complexes. These ligands, derived from N-(1-naphthyl)ethylenediamine and various phenol aldehydes, feature multiple coordination sites that facilitate diverse structural arrangements and tunable physicochemical properties [1].

In this study, a series of novel Schiff base ligands were synthesized, utilizing N-(1-naphthyl)ethylenediamine and various phenol aldehydes. These imino ligands and the amino derivatives obtained by reduction were used either alone or in combination with other chelating ligands to generate both mono- and multinuclear complexes. Single-crystal X-ray diffraction was employed to structurally characterize the ligands and complexes, revealing the versatility of these imino and amino derivatives and showing the coordination geometries and organization of the complexes. Figure 1 shows the schematic synthesis of a Zn(II) complex using the aforementioned type of ligands.

Furthermore, the study analyzed the optical properties of the synthesized ligands and complexes in the solid-state through various types of spectroscopies. The luminescence properties of these complexes were of particular interest due to the extended  $\pi$ -systems of the ligands, which are capable of enhanced fluorescence emission.

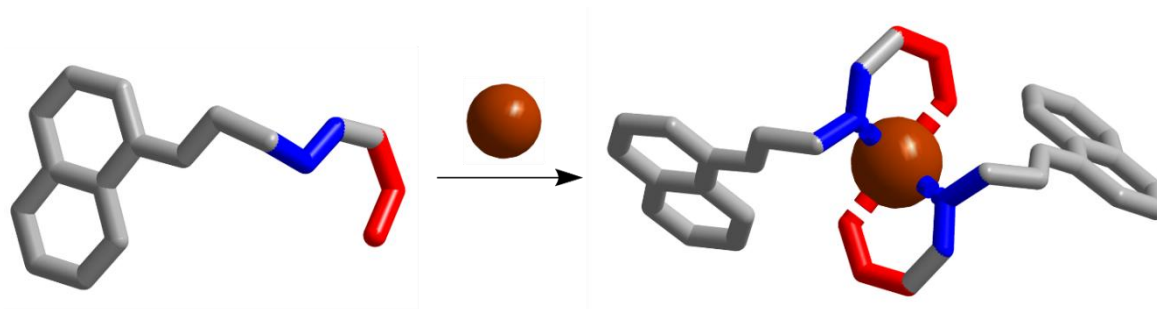


Figure 1: Schematic synthesis of 3d complexes using Schiff base ligands.

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## O16 Study on the Reactivity of Organobismuth(I) Compounds Towards *ortho*-quinones

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Bismuthinidenes are a class of organobismuth(I) compounds analogous to carbenes. However, due to their low oxidation state, they are highly reactive and unstable. Over the past decade, these bismuth(I) compounds have been studied for their intriguing transition metal-like behavior and their ability to undergo oxidative addition to various substrates, including aliphatic compounds (such as alkyl iodides and triflates) and aromatic compounds (such as diazonium salts). This opens the possibility of employing bismuth, a main group metal, in redox catalysis. Recently, there has been growing interest in reactions between heavier carbene analogues and quinones due to the intriguing redox properties of the latter. The Lichtenberg's research group, for instance, used *ortho*-quinones to trap a bismuth(I) intermediate and further investigate CO<sub>2</sub> and CS<sub>2</sub> insertion into bismuth-nitrogen bonds [1]. Additionally, their reactivity towards arsinidenes and stibinidenes has been recently explored [2]. Starting from this background the main objective of this work aims to evaluate the reactivity and to elucidate the reaction mechanisms of a *cyclo*-organobismuth(I) compound with *ortho*-quinones.

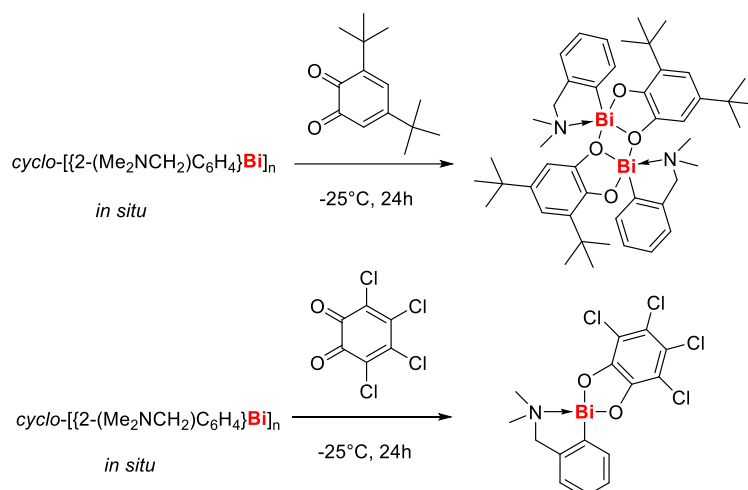


Figure 1: Reaction of an organobismuth(I) compound with two different *ortho*-quinones.

**Acknowledgements:** This research was supported by Technische Universität Chemnitz.

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## **O17 Morphological Features Dictate Drug Release from Nanostructured Borosilicate – Alginate Aerogels and Xerogels**

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Aerogels are the world's lowest-density solids with an open and coherent mesoporous structure, and in 2022 they were included in the IUPAC's "Top Ten Emerging Technologies in Chemistry" list. This is because their application offers innovative solutions for a wide range of applications. These include space, construction, and biomedical applications [1].

In our research, we have successfully synthesized borosilicate-alginate composite gels, from which xerogels and aerogels were prepared by different drying methods. The model drug, nicotinic acid was successfully impregnated into these samples by different impregnation strategies. The chemical composition of the solid gels was investigated by infrared spectroscopy, their morphology by scanning electron microscopy and N<sub>2</sub> adsorption-desorption porosimetry, and information on their crystallinity was obtained by XRD measurements.

The different formulation technologies resulted in dramatically different aero- and xerogel based drug delivery systems. For aerogels, the drug was impregnated in an amorphous form, which, in combination with large pores, results in rapid and highly efficient drug release, which can be beneficial for poorly water-soluble drugs. The release from xerogels is more prolonged and retarded. Xerogels dried from the mother liquor have the highest dosage, and the crystalline form of the drug together with the denser structure of the xerogels result in a prolonged release.

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## O18 Photophysical Studies on Thin Films of Hybrid Liquid Crystalline Materials Based on an Emissive Metallomesogen

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Research into luminescent hybrid liquid crystalline materials has progressed significantly in recent years, particularly those formed by dispersing various optically active nanomaterials into liquid crystalline (LC) phases. These materials are gaining attention due to their unique properties, which have potential applications in fields like biomedicine [1] and LCDs [2]. We recently reported on hybrid materials obtained from metallomesogens and carbon-based nanomaterials (such as CNTs and graphene) that can be used as paste electrodes for the non-enzymatic electrochemical detection of various analytes [3].

Here we will present a new luminescent hybrid system (MIX) that combines a room-temperature metallomesogen (Zn\_MM) with N-doped carbon dots. The Zn\_MM is based on a terpyridine ligand and 3,4,5-trialkyl substituted gallate co-ligands [4]. The hybrid material was obtained by ultrasonically mixing the components (Figure 1). The emissive properties of the final hybrid materials were investigated by spectroscopic and optical methods.

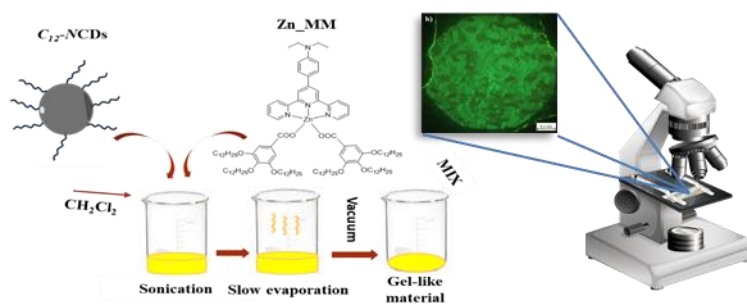


Figure 1: Schematic representation synthesis of luminescent hybrid LC system (left) and POM micrograph of MIX (right).

**Acknowledgment:** We acknowledge the Romanian Academy, Program 4, and the project ROOPENSCREEN, MySMIS code: 127952, Contract no. 371/20.07.2020, co-financed by European Regional Development Fund through the Competitiveness Operational Program 2014-2020, for support.

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## **O19 Synthesis and Electrochemical Testing of Polyacrylic Acid Based Hydrogel Electrolyte for Zn–air Battery**

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Innovative energy storage solutions are one of the most pressing issues of our time. In addition to lithium-ion batteries, metal–air batteries are becoming increasingly important, with the advantage of containing a higher abundance of metal than lithium, being easier to handle, less expensive and safer. An alkaline Zn-air battery with charcoal cathode and zinc anode has been developed at the Department of Applied Chemistry of the University of Debrecen [1] [2]. However, in addition to cathode and anode development, electrolyte development is also important. In my research, I aimed to develop a polymer-based hydrogel electrolyte. Polyacrylic acid is an easily cross-linkable polymer with a high degree of swelling, which is used in a wide range of applications from agricultural water binders to medical devices [3] [4] [5]. Cross-linked polyacrylic acid was prepared by a radical polymerization reaction with ammonium persulfate (APS) initiator and *N,N'*-methylene-bis-acrylamide (MBAA) cross-linker [6]. The gels were prepared in 3D printed PETG molding vats of our own design and fabrication. The gels were swelled in different solutions with different concentrations of ZnO (0.05 M - 0.25 M) and KOH (2 M - 6 M). We also varied the concentration of MBAA crosslinker (0.05 - 0.75 mol%), which was later finalized in 0.25 mol% MBAA. In addition, cell assembly was also performed. The anode was a zinc plate, the electrolyte was a crosslinked polyacrylic acid (0.25 mol% MBAA crosslinker, 0.1 mol% APS initiator) expanded in ZnO+KOH solution, while the cathode was activated carbon coated on Ni-foam with PVDF binder. The cell was also subjected to cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS) and charge–discharge studies. The latter showed that the cell still operated with a potential gap of 0.4 V after 20 h (30 min/cycle; 2 mA current), while the Coulomb efficiency was still close to 100%.

**Acknowledgements:** Thank you to the following applications for financial support in this work: The project NKFI FK-147503, RRF-2.3.1-21-2022-00009, National Renewable Energy Laboratory, was implemented under the Széchenyi Plan Plus programme with the support of the European Union's Instrument for Recovery and Resilience. It was also supported by the University of Debrecen under the University Research Fellowship Programme EKÖP-24-3-II-DE-110. Thanks for the financial support provided by the MOL Group, Hungary.

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## O20 Thermoresponsive LCST-type Random Copolymers with PEG Methyl Ether Methacrylate of 1100 g/mol Molecular Weight: The Effect of Composition and the CST of the Homopolymers

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The thermoresponsive behavior of copolymers based on PEG-methyl ether methacrylate with a molecular weight of 1100 g/mol (mPEGMA<sub>1100</sub>) was investigated. The ability to fine tune the critical solution temperature (CST) is of utmost importance in order to exploit their immense potential in a wide range of applications. A library of mPEGMA<sub>1100</sub> based copolymers was prepared with varying comonomer ratios using four main widely used and available comonomers, namely: *N*-isopropyl acrylamide, *N*-isopropyl methacrylamide, di(ethylene glycol) ethyl ether acrylate and mPEGMA<sub>300</sub> having different CST values.

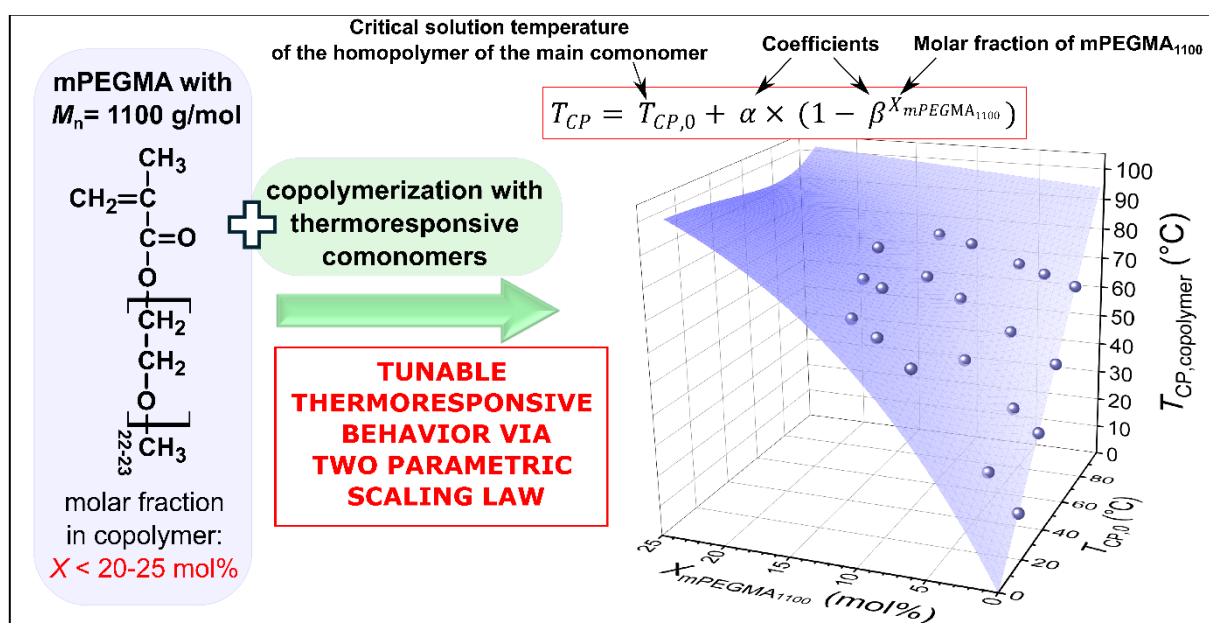


Figure 1: The two-parameter scaling law and the 3D plot of the  $T_{CP}$  values of the mPEGMA<sub>1100</sub> based copolymers as a function of mPEGMA<sub>1100</sub> content and the CST of the comonomer ( $T_{CP,0}$ )

It was found that a relatively small amount of mPEGMA<sub>1100</sub> was sufficient to adjust the CST of the copolymers up to 100 °C. Additionally, a predictive asymptotic function-based model was developed, which revealed that the CST of the copolymers depends only on the PEG content and the CST of the main comonomer. This model defines a 3D surface which allows to determine the CST of copolymers in advance or to define a suitable composition for a desired CST, enabling the design of a variety of novel macromolecular structures with fine-tuned thermoresponsive properties.

**Acknowledgments:** National Research, Development and Innovation Office, Hungary (grant numbers PD139162, K135946 and TKP2021-EGA-31).

## **O21 Defects Induced by Lithium in ZnO Nanorods Used for Supercapacitor Applications**

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Significant research efforts have been dedicated toward developing environmentally friendly energy storage technologies as a result of the growing demand for ecologically sustainable energy and the rapid depletion of existing fossil fuels. Besides batteries and capacitors, a modern device has emerged, the supercapacitor (SC) trying to combine both the properties of batteries and capacitors [1]. A SC consists of four major components: electrodes, electrolytes, separators and collectors, and among these the electrode material is the most tailored to improve the SC's performance [2]. In this study, ZnO nanorods, synthesized using the hydrothermal method, were doped with several lithium concentrations and were studied as electrode material for SC devices in order to find out the benefits created by lithium-induced defects in the ZnO structure. The samples were thoroughly characterized by scanning/transmission electron microscopy, X-ray diffraction, and spectroscopic techniques like photoluminescence, UV-vis, Raman, and electron paramagnetic resonance spectroscopy. Subsequently, the ZnO-based materials were assembled in symmetric supercapacitor devices to test their energy storage capabilities. The maximum specific capacitance was achieved for the 0.5% Li-doped ZnO, which showed a value of 700 F/g at 1 mV/s with an impressive energy density of 56 Wh/kg and excellent cyclic stability.

*Acknowledgements:* This work was supported through the Ministry of Research, Innovation and Digitalization, Romania's National Recovery and Resilience Plan, PNRR-III-C9-2022-I8, CF 163/15.11.22, financing contract no. 760097/23.05.23.

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## **O22 The Modification of Nanocellulose with a Sulfated Polysaccharide: A Physico-Chemical Study**

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Brown algae are the largest biomass producers in coastal sea regions and a source of valuable polysaccharides [1]. Fucose-containing sulfated polysaccharides including fucoidans are important components of brown algae, which are currently extensively studied for biomedical applications, due to their antioxidant, anti-inflammatory, antiviral, antiglycemic, and anticancer activities [2]. However, the application of fucoidan (F) in medical, pharmaceutical, or food industries is quite limited due to the complexity and high costs of extraction and purification processes, its low viscosity, and lack of gelling ability [3]. Nanocellulose (NC) can serve as a stabilizing agent, a drug carrier, or a scaffold in tissue engineering due to its high surface area, biodegradability, biocompatibility, and high mechanical strength [4]. Loading NC with F could cumulate the valuable properties of both natural products, leading to antidiabetic or antiviral drugs, food additives, scaffolds, or dressings with anti-inflammatory features.

In this work, a fucoidan extracted from brown seaweed was physico-chemical characterized by Fourier-transform infrared spectroscopy (FTIR), sulfate content, and thermogravimetric analysis (TGA), and used in different formulations with a nanocellulose obtained from microcrystalline cellulose by mechanical treatment. The formulations with different NC/F ratios were characterized by FTIR, scanning electron microscopy, TGA, and dynamic mechanical analysis for studying the effect of F on the properties of nanocellulose.

The results show that fucoidan has no significant influence on the nanometric size of NC, but the NC/F ratio influenced the thermal and mechanical characteristics of the modified nanocellulose.

*Acknowledgements:* This work was supported by a grant of the Ministry of Education and Research, CNCS - UEFISCDI, project number PN-IV-P1-PCE-2023-1557, contract 37PCE/2025 (WASTE2COAT) within PNCDI IV and project PN23.06.01.01/2022 AQUAMAT, within PN23.06 Core Program-ChemNewDeal.

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## **O23 Coordination Chemistry Behaviour of Cu(II), Zn(II) and Ni(II) with Some Native and Phosphorylated Tau Protein Peptides**

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Taupathies are one the major forms of neurodegenerative disorders, of which Alzheimer's disease is the best known and most common. It has a big association with the accumulation of hyperphosphorylated tau protein in the form of neurofibrillary tangles [1]. Tau protein plays an important role in the stabilization of microtubules of the nervous cell, and the interaction between metal ion and the protein fragments plays an important role in the accumulation process, but the exact mechanism of these accumulation processes still not satisfactorily clear [2].

The specific phosphorylation of Serine262 and Serine356 in tau protein by MARK kinase enzymes have been described to decrease the microtubule binding affinity of tau protein for microtubules, and the phosphorylation of this protein is associated with the destabilization of the tau microtubule complex and the assembly of tau protein into toxic aggregates and metal ions have a significant impact on this process [3].

In our work, we synthesized tau(262-270): Ac-STENLKHQP-NH<sub>2</sub> peptide by solid phase peptide synthesizer, we studied the coordination chemistry behaviour of this peptide with three metal ions [Cu(II), Ni(II) and Zn(II)] and also the loner peptide sequence tau(258-270) Ac-SKIGSTENLKHQP-NH<sub>2</sub>. In order to clearly see the impact of phosphorylation of serine on the complex formation process, we also studied the coordination chemistry behaviour of its serine phosphorylated versions with the same metal ions. The complex formation process of all peptides were thoroughly described. In case of all these peptides, histidyl residues are anchoring groups which are responsible for coordinating to the metal ion and further amide nitrogen atoms are also bond in the basic solution.

In this presentation will be shown how the phosphorylation of serine in different positions affects the stability and coordination of metal complexes of peptides.

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## **O24 Intraprotein Electron Routes in Ascorbate/Caffeate - Myoglobin Systems**

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An exhaustive evaluation of electron routes within myoglobin is reported here by employing the Non-Equilibrium Greens Function coupled with Density Functional Theory (NEGF-DFT) formalism. The obtained results provide a higher resolution for evaluating electron paths in proteins than the usually encountered Marcus Theory based methods.

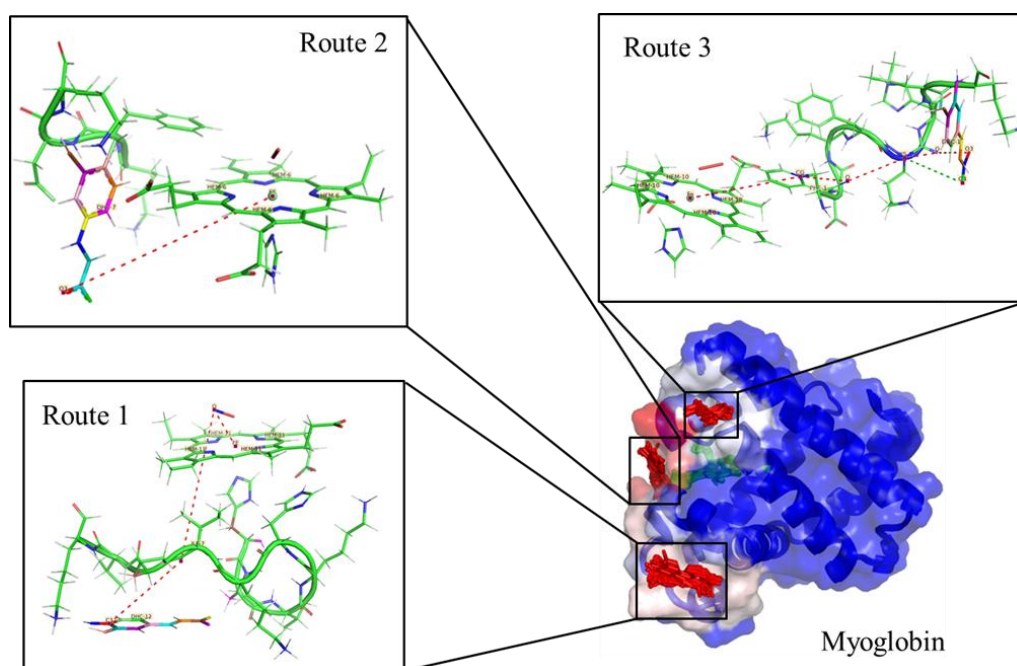


Figure 1: Electron transfer routes from myoglobin's caffeate binding sites toward its catalytic heme iron.

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The computational facilities were provided by the CLOUDUT Project, co-funded by the European Fund of Regional Development through the Competitiveness Operational Programme 2014-2020, contract no. 235/2020.

## **O25 Structural Aspects in Organotin(IV) Selenolates**

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Organotin(IV) compounds have attracted considerable interest over the last few years due to their potential biological properties (as antibacterial or antitumor agents) and their applications as precursors for nanomaterials in optoelectronics. On the other hand, various organoselenium compounds have been intensively studied for their antioxidant and antiproliferative properties, and they have also been utilised as immunomodulators, anti-inflammatory agents, and antidepressant drugs [1,2]. Our recent research interest was focused on the synthesis and structural characterization of organotin compounds with organoselenolato ligands with potential for biological applications or potential candidates for CVD processes. To increase the stability of the organotin compounds, we used aromatic organic groups bearing pendant arms with nitrogen donor atoms capable of N→E intramolecular interactions, e.g. 2-(Me<sub>2</sub>NCH<sub>2</sub>)C<sub>6</sub>H<sub>4</sub>.

We report here on the synthesis and structural characterisation of several homo- and heteroleptic diorganotin(IV) and triorganotin(IV) complexes with organoselenolato ligands of type pzCH<sub>2</sub>CH<sub>2</sub>Se<sup>-</sup> (pz = pyrazole). Compounds of type RR'Sn(SeCH<sub>2</sub>CH<sub>2</sub>pz)<sub>2</sub> (R = 2-(Me<sub>2</sub>NCH<sub>2</sub>)C<sub>6</sub>H<sub>4</sub>; R' = Me, <sup>n</sup>Bu, Ph) were prepared by reacting RR'SnCl<sub>2</sub> with Na[SeCH<sub>2</sub>CH<sub>2</sub>pz] in a 1:2 molar ratio. Similarly, was prepared the compound [2-(Me<sub>2</sub>NCH<sub>2</sub>)C<sub>6</sub>H<sub>4</sub>]SnCl(SeCH<sub>2</sub>CH<sub>2</sub>pz), when a 1:1 molar ratio was used.

The diorganotin(IV)pseudohalido organoselenolates RR'Sn(NCS)(SeCH<sub>2</sub>CH<sub>2</sub>pz) (R = 2-(Me<sub>2</sub>NCH<sub>2</sub>)C<sub>6</sub>H<sub>4</sub>; R' = Me, <sup>n</sup>Bu, Ph) were prepared by reacting the Na[SeCH<sub>2</sub>CH<sub>2</sub>pz] in a 1:1 molar ratio with RR'Sn(NCS)<sub>2</sub> (R = 2-(Me<sub>2</sub>NCH<sub>2</sub>)C<sub>6</sub>H<sub>4</sub>; R' = Me, <sup>n</sup>Bu, Ph). All compounds were characterized by multinuclear (<sup>1</sup>H, <sup>13</sup>C{<sup>1</sup>H}, <sup>77</sup>Se{<sup>1</sup>H}, <sup>119</sup>Sn{<sup>1</sup>H}) NMR experiments and mass spectrometry.

*Acknowledgements:* The financial support of UEFISCDI, project no. PN-IV-P1-PCE-2023-0966 is highly acknowledged.

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## **O26 Synthesis, Structural Characterization and Reactivity of New Pyridine Based Organoselenium Compounds**

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Organoselenium compounds have undergone significant development in the past decade in several fields such as biology, catalysis or materials science. The research shows that the presence of additional nitrogen donor atoms capable of coordination can influence the stability of the organoselenium species, but, more important, their reactivity and specific behavior in the fields mentioned above [1,2].

Here in, we report on the synthesis and structural characterization of some new pyridine based diorganoselenides (Figure 1). The coordination ability of such ligands was investigated towards silver and copper.

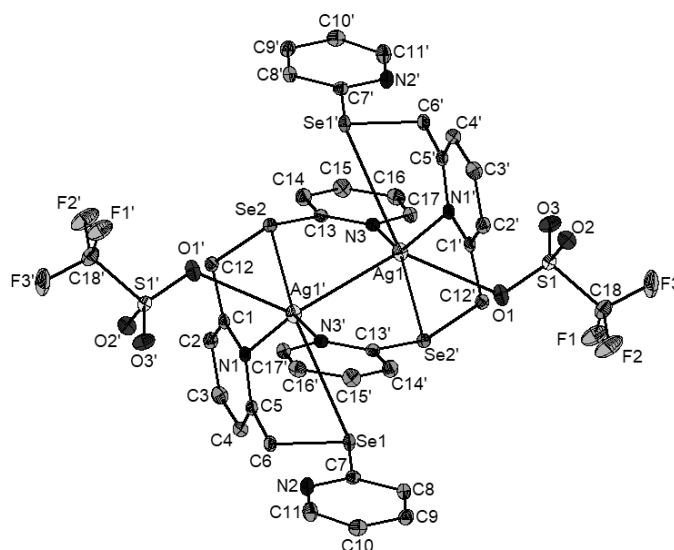


Figure 1: Organoselenium pyridine based compound.

The ligands and their metal complexes were investigated by multinuclear NMR spectroscopy ( $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{77}\text{Se}$ ,  $^{31}\text{P}$  and  $^{19}\text{F}$ , as appropriate), mass spectrometry, molar conductivity and UV-Vis spectroscopy. The molecular structures of representative compounds were determined by single-crystal X-Ray diffraction.

*Acknowledgements:* This work was supported by the UEFISCDI (Project PN-IV-P1-PCE-2023-0966).

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## **O27 Metal Binding Ability of Tau (289-300) Fragment**

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Taupathies including Alzheimer's disease (AD) are a group of neurodegenerative disorders characterized by decline in cognitive abilities. Its development is associated with the accumulation of extracellular amyloid- $\beta$  plaques and hyperphosphorylated tau protein leading to the formation of intracellular neurofibrillary tangles [1], [2]. The metal dyshomeostasis plays an important role where the concentration of zinc, iron and copper increases in neuron resulting in conformational changes and aggregation of tau protein [3]. Tau mostly binds through the 2 cysteine or 12 histidine residues present in its sequence, which are the most common metal binding sites [4].

For further elucidation of these binding sites we investigated the tau fragment with Cys 291 and His 299 (tau 289-300; Ac-SKCGSKDNIKH<sub>2</sub>NH<sub>2</sub>) in the sequence. In addition to this, tau fragments containing only Cys 291, tau 288-293; Ac-QSKCGS-NH<sub>2</sub> and tau 289-292; Ac-SKCG-NH<sub>2</sub>, and only His 299; tau 292-301, Ac-GSKDNIKHVP-NH<sub>2</sub> and its asparagine mutant at position 300 were synthesized and their coordination and electrochemical properties were studied.

The pH potentiometric titrations for the above five ligands and their Ni(II) complexes were performed. We observed that for Cys containing fragments (tau(289-292) and tau(288-293)), as the pH was increased, [NiLH<sub>-2</sub>] complexes form as a major species where the Ni<sup>+2</sup> ion is coordinatively saturated at all the four sites by thiol group and the 3 deprotonated amide nitrogen as [N<sup>-</sup>,N<sup>-</sup>,N<sup>-</sup>,S<sup>-</sup>]. The lysines are deprotonated on further increase in pH but not coordinated to the metal ions. The study of Ni<sup>+2</sup> and Cu<sup>+2</sup> complexes of His containing ligands (tau(292-301)) a four-coordinated complex was observed as major species, in which metal ions are coordinated by the histidine imidazole N and 3 amide N. These results were supported by the UV-vis and circular dichroism spectroscopic studies. The data also inferred that the mutation of an uncoordinated amino acid, Val to Asn in fragment has little effect on stability constant and no significant effect on the binding mode of metal ions to the tau fragment.

The comparative analysis of stability constants of metal complexes of all the peptides showed that, the peptide containing both His and Cys are more stable than peptides containing only His, concluding that if present in the sequence, Cys takes part in coordination with the metal ion. The spectrophotometric and CD curves of Ni(II) complexes showed a clear shoulder peak characteristic of Ni-S binding in fragments containing cysteine, which was not observed in tau fragments containing histidine alone, indicating that Cys is a preferred binding site for Ni(II) in tau fragments where both Cys and His are present in the sequence.

*Acknowledgements:* The research was supported by the University of Debrecen Program for Scientific Publication and the University of Debrecen Scientific Research Bridging Fund (DETKA).

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## **O28 Hybrid Supramolecular Ordered Materials Based on Metallomesogens for Electrochemical Sensing**

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Modern materials science relies greatly on hybrid materials but faces substantial challenges in achieving compositional reproducibility [1]. Liquid crystals deliver dynamic optical and structural characteristics and can be used to integrate inorganic nanoparticles yielding controllable supramolecular ordered hybrid materials [2,3]. These systems may show significant potential for use in sensor technology, optoelectronic devices, and photonic applications. The stability and performance of the final material alongside its uniformity depend on the complex problem of controlling carbon dot dispersion within the liquid crystal matrix. Optimization of synthesis protocols through further research combined with advanced characterization techniques will improve material uniformity leading to consistent performance in applications.

Herein the synthesis and characterization of hybrid materials based on metallomesogens and silver carbon dots (CDs@Ag) will be presented. A room temperature metallomesogen based on Cu(II) metal center arranging into columnar hexagonal mesophase has been chosen [4]. Carbon dots were synthesized by microwave method and were used to obtain CDs@Ag [5]. The final hybrid materials were obtained by blending and were characterized by spectroscopic and microscopic methods, while their supramolecular order was evidenced by diffraction studies. Preliminary electrochemical behaviours in different supporting electrolyte envisaging their use as voltammetric/amperometric sensor will be presented.

*Acknowledgements:* We acknowledge the Romanian Academy, Program 4 for support.

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**POSTER PRESENTATIONS**

**P1 – P17**

## **P1 Monitoring Reaction Kinetics in the Determination of Antioxidant Activities of Phenolic Compounds**

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Phenolic compounds, representatives of plant secondary metabolites, are known to be one of the most important classes of natural antioxidants, whose intensity of antioxidant effect depends on their structural properties. They are attracting increasing attention due to their impact on health, and it is desirable to study their reaction with factors that promote oxidative stress [1-3]. Thus, monitoring reaction kinetics is essential to understand their antioxidant capacity and how they interact with reactive species [4]. The work aimed to monitor the reaction kinetics between phenolic compounds from different classes and the DPPH• (2,2-Diphenyl-1-picrylhydrazyl) radical, using the UV-Vis spectrophotometric method. In the experimental part, the ratio between DPPH• radical solution and solutions of phenolic acids and flavonoids was kept at 1:1, at a concentration of 0.25 mM. Subsequently, by adding the antioxidant solutions and the free radical, the decrease in absorbance was continuously monitored until the stabilization of the reaction, and kinetic data analysis was performed in triplicate to validate the reproducibility of the measurements. The experimental results indicated that the reactions follow second-order kinetics, and the values of rate constants and half-life vary significantly depending on the molecular structure of each compound. Thus, the influence of the number and arrangement of hydroxyl functional groups (-OH) on the efficiency of the radical neutralization process is highlighted. This variation emphasizes the influence of structural parameters on the reaction rate and antioxidant efficiency. It also confirms the importance of monitoring the kinetics of the reaction with the DPPH• radical to evaluate the antioxidant potential of phenolic compounds, contributing to the further understanding of their mechanisms of action.

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## **P2 Encapsulation of Anthocyanins from *Vaccinium Vitis-Idaea* Extracts**

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Lingonberries (*Vaccinium vitis-idaea*) are one of the most important harvested wild berries from temperate climate zones. These fruits contain a large variety of different polyphenolic compounds such as anthocyanins, flavonols, and phenolic acids, also being popular for the antioxidant properties [1]. Due to high amount of organic acids, especially citric acids, the flavor of lingonberries is very acidic and sour [2].

Anthocyanins are natural pigments of the flavonoid class, responsible for the red, purple and blue color of many fruits and vegetables. In lingonberries, anthocyanins contribute significantly to their characteristic red color and antioxidant activity. However, anthocyanins are sensitive to environmental factors such as pH, temperature and light, which limits their stability and applicability in the food industry [3].

The aim of this study was to extract anthocyanins from *Vaccinium vitis-idaea* and to determine the total anthocyanins content with a spectrophotometric differential pH method to quantify their concentration, followed by their encapsulation in liposomes. Furthermore, the study evaluated the encapsulation efficiency, the residual anthocyanin content, and the interaction between anthocyanins and the encapsulating agents.

The encapsulation of lingonberry anthocyanins in lecithin liposomes protected these compounds from degradation factors such as pH, temperature and light thus contributing to maintain stability. This method also improved the solubility and dispersibility of anthocyanins in aqueous solutions, facilitating their use in food and pharmaceutical applications.

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### **P3 No Heme-Chlorite Adduct in the Catalytic Cycle of Chlorite Dismutase: Insights From QM/MM and Dynamics Calculations**

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Chlorite dismutase (Cld) is one of the rare enzymes capable of forming oxygen-oxygen bonds. Cld has been identified in a very small number of anaerobic bacteria that can use perchlorate as the final electron acceptor in their electron transport/respiration chain. It has been proposed that the catalytic cycle of Cld involves the binding of chlorite to the enzyme's active site, followed by the cleavage of one of the Cl-O bonds, leading to the formation of a high-valent iron-oxo center and a ClO radical/ion, and then a reorientation to the oxygen atom bound to iron, followed by the release of chloride and molecular oxygen. However, direct experimental confirmation of the existence of a chlorite-heme adduct in Cld is still unavailable, nor is it clear what the coordination mode of chlorite is. Moreover, reaction intermediates have not been directly observed in experiments. Previous DFT calculation from us and others have concluded that hemes cannot form stable adducts with chlorite – unlike, e.g., metallacorrins such as cobalamin [1]. This paper the results obtained from QM/MM optimization and QM/MM molecular dynamics calculations on the catalytic cycle, revealing compelling computational evidence that a chlorite-heme adduct in Cld is unlikely to be observable experimentally.

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## P4 New Analytical Methods for Quantification of Hg Species in Soft Water Using HPLC-ICP-MS Technique

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Mercury is a highly toxic element with negative effects on the environment and human health due to its bio accumulative properties. Although ecological impact assessment and health risk evaluations typically consider only the total Hg content, it is crucial to distinguish between the highly toxic alkylated mercury compounds (primarily methylmercury, MeHg) and the less toxic inorganic forms of mercury [1].

The aim of this study was to develop, optimize, and validate an analytical method for simultaneous quantification of mercury species ( $\text{Hg}^{2+}$ , MeHg) in soft water (drinking water, surface water, groundwater) using HPLC-ICP-MS spectrometry. The experimental tests were performed using an Agilent 1260 Infinity II HPLC system coupled with an Agilent 7850 ICP-MS. A Thermo Scientific Hypersil Gold column (150 mm  $\times$  4.6 mm) was used at ambient temperature. L-cysteine (solution 1 g/L) at a flow rate of 1.0 mL/min was used as mobile phase. The time for a sample was 7 minutes. A five-point calibration curve was established for both  $\text{Hg}^{2+}$  and MeHg within the concentration range of 0.1 to 1.0  $\mu\text{g/L}$  (Figure 1). For both organic and inorganic mercury, measurements were taken for 199, 200, 201, and 202 isotopes.

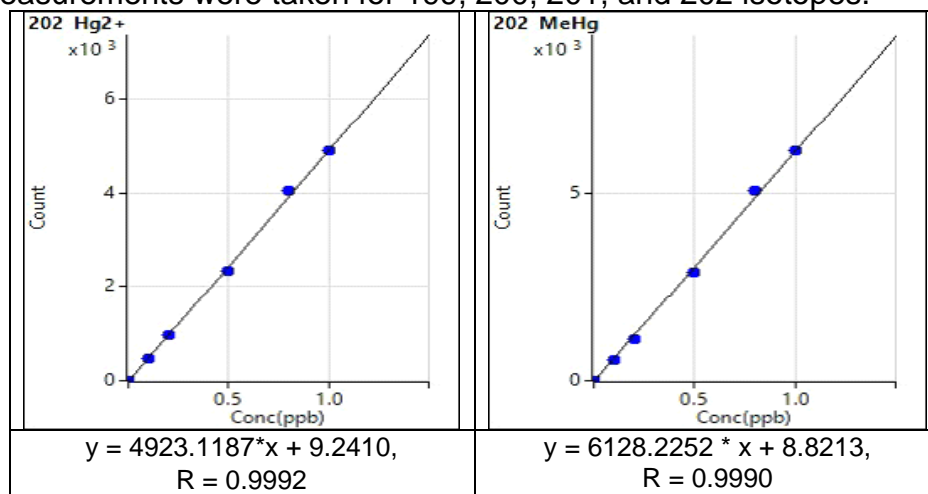


Figure 1: Calibration curves for  $\text{Hg}^{2+}$  and MeHg at 1  $\mu\text{g/L}$

The quantification limits ranged between 0.10  $\mu\text{g/L}$  and 0.11  $\mu\text{g/L}$ . Recovery percentage were situated from 52.4% to 112.7%. The best results were obtained for  $^{202}\text{Hg}^{2+}$  and  $^{202}\text{MeHg}$ . The results confirm the capability of the method to quantify mercury species in drinking water, surface water, and groundwater samples.

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## **P5 LC-MS/MS Method for the Determination of Perfluoroalkyl Sulfonic Acids in Dehydrated Sludge from Wastewater Treatment Plants**

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PFAS in wastewater treatment plants (WWTPs) mainly originate from direct release of PFAS-containing products (food packaging, cosmetics, etc.), domestic wastewater, and in situ formation of PFAS from PFAS precursors present in wastewater [1]. Conventional WWTPs do not have specific treatment/disposal processes for the treatment and removal of PFAS.

The aim of the study was to develop and validate a simultaneous method for the determination of PFAS compounds in sewage sludge samples. An Avantor ACE PFAS Delay column (10 x 2.1 mm, 2.0  $\mu$ m) and an Avantor ACE HTP-MS precolumn (50 x 2.1 mm) were used. The mobile phase used was 2 mM ammonium acetate solution mixed with 2 mM methanol. The optimized flow rate of the mobile phase was 0.4 mL/min. After optimization of the LC-MS/MS parameters, the linear range was established in the range of 0.02  $\mu$ g/g to 0.06  $\mu$ g/g. The optimized conditions of the chromatographic parameters allowed the separation of 30 PFAS compounds in 15.5 minutes (Figure 1).

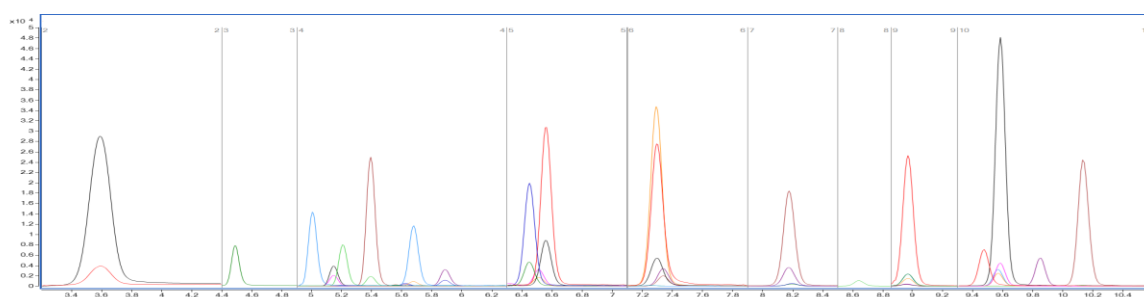


Figura 1: MRM Chromatograms for PFAS at 0.02  $\mu$ g/g

The quantification limits (LOQ) were situated between 0.011  $\mu$ g/g to 0.037  $\mu$ g/g. Repeatability tests indicated RSD values between 1% and 5%. The treatment of sewage sludge samples was carried out by ultrasound-assisted extraction with recovery percentage higher than 75%. The results obtained on real samples indicated that PFAS compounds are present in the sludge, but at levels below the LOQ, suggesting the efficiency of the selected treatment systems.

**Acknowledgements:** This work was carried out through the “Nucleu” Program within the National Research Development and Innovation Plan 2022-2027 with the support of Romanian Ministry of Research, Innovation and Digitalization, contract no. 3N/2022, Project code PN 23 22 01 01.

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## **P6 Polyacrylic Acid Gel-Based Electrolytes for Rechargeable Zn-Air Batteries**

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Zinc-air batteries are one of the most promising energy storage systems due to their excellent theoretical specific energy. Zinc-air batteries (ZABs) have been developed to provide constant power for new wearable and portable electronic devices due to their potential biocompatibility and low production cost. However, the spread of these batteries is hampered by their poor recyclability, the formation of dendritic deposits and the passivation of the anode. These challenges are closely related and an integrated strategy is required to find a suitable solution. Aqueous electrolytes have some limitations such as carbonation, leakage and water loss, which adversely affect battery performance. Polymer-based gel electrolytes have shown advantages over the limitations for ZABs, these include dendrite reduction, interfacial stabilisation of the phases, little or no electrolyte leakage. This work focuses on the development of a polyacrylic acid gel electrolyte to determine its optimum conductive performance in ZABs by varying the concentrations of cross-linking agent (*N,N'*-methylene-bisacrylamide), potassium hydroxide (KOH) and zinc oxide in the prepared gel electrolyte. Impedance spectroscopy was used to determine the performance of the electrolytes. In addition, the electrolytes were tested in batteries and the effect of the electrolyte properties on cycling performance, Coulomb and energy efficiency was investigated.

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## **P7 Rapid Synthesis of Thermoresponsive PNIPA-*b*-PNAM Block Copolymers**

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Synthesis of multiblock copolymers with controlled molecular weight and low dispersity is a challenging endeavor. Copolymers of *N*-isopropylacrylamide and *N*-acryloylmorpholine display thermoresponsive behavior owing to the presence of pNIPA. The pNIPA contains hydrophilic amido group and hydrophobic isopropyl group in its repeating unit that provides lower critical solution temperature (LCST) phase behavior in aqueous solution [1]. The reported synthesis of copolymers usually involves long reaction times and sometimes with poor control over dispersity [2]. Herein, we report a rapid one pot synthesis with considerably less reaction time of about 20 mins per block employing a Reversible Addition-fragmentation Chain transfer (RAFT) polymerization. Our method is particularly useful when low degree of polymerization (DP < 50) is targeted. The Chemical structure of copolymers as analyzed by Matrix-Assisted Laser Desorption/Ionization (MALDI) mass spectrometry revealed the presence of peaks differing by approximately 28Da confirming the presence of pNIPA-*b*-pNAM copolymers. To determine the copolymer composition from a single MS measurement, a novel and efficient method that fits peak curves to the raw data was developed [3]. From the fitting parameters, the accurate composition of the copolymer can be established. One of the main advantages of our method is the identification of the distribution of the monomers in a copolymer.

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## **P8 Synthesis and Study of Multiblock Copolymers of Acrylamide Derivatives**

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The preparation of functional block copolymers is often considered a synthetic challenge from a polymer chemist's point of view. Reversible addition-fragmentation chain transfer (RAFT) polymerization is an effective method for the synthesis of these compounds [1]. The properties of block copolymers can be effectively controlled by the chemical composition of the copolymers, which includes the monomer quality and their ratio. As such, they can offer a wide range of applications in the pharmaceutical industry as potential drug carriers and in materials science [2]. We have prepared poly(*N*-acryloylmorpholine)-block-poly(*N*-isopropylacrylamide) (pNAM-b-pNIPAM) copolymers with variable block lengths of 2-6 blocks. The block copolymers were purified before addition of the new block. A detailed analysis of these complex systems can be performed by mass spectrometry methods, but the evaluation is challenging due to the large number of peaks expected in the spectra and their overlapping. The prepared multiblock copolymers are measured by MALDI-TOF mass spectrometry. We determined the degree of polymerisation of the blocks, polydispersity and number average molecular weight for all the copolymers. For the evaluation of the spectra we used our novel algorithm where the key steps are the calculation of all possible compounds and the fitting of the distribution of the two monomer units. In addition, we investigate the self-assembly properties of these systems using dynamic light scattering (DLS) experiments to explore the relationships between copolymer characteristics and phase transition temperature. In this way, the aggregation behaviour of the designed copolymer can be estimated. By producing diblock copolymers with variable combinations, I aimed explore structure property relationships among the copolymer characteristics and their thermal behaviour.

*Acknowledgements:* Thank you to the following applications for financial support in this work: The project NKFI FK-147503, RRF-2.3.1-21-2022-00009, National Renewable Energy Laboratory, was implemented under the Széchenyi Plan Plus programme with the support of the European Union's Instrument for Recovery and Resilience. It was also supported by the University of Debrecen under the University Research Fellowship Programme EKÖP-24-3-II-DE-130. Thanks for the financial support provided by the Mol Group, Hungary.

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## **P9 Design and Synthesis of Poly-Functionalized Azides for “click” Chemistry-Based Microscopy Applications**

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Azides are important compounds in both organic synthesis, as precursors of other functional groups, such as amines and heterocycles [1], and in the design and synthesis of polyfunctionalized molecules, such as amino-azide, with diverse applications in biomedicine [2,3]. Most prominently, azides react with terminal alkynes via the Cu(I)-catalyzed Azide-Alkyne Cycloaddition reaction (CuAAC, Figure 1) [4,5], a key tool for accessing a seemingly limitless number of complex molecules and structures, with unparalleled efficiency and selectivity.

The unique advantages offered by the CuAAC reaction have led to various organic azides being designed for numerous applications in chemistry, biochemistry, cell biology and medicine, such as microscopic imaging, preparation of antibody conjugates, or diagnostic tests [2,3].

In this context, we present synthetic strategies for the preparation of several key amino-azide precursors, including optimization of reaction steps and optimal choices for groups. Confirmation of the target structures by spectral analysis (NMR, HRMS) is also provided. We anticipate that the compounds hereby reported will be useful in various biological applications that use CuAAC for microscopic imaging of cells and tissues.

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## P10 Synthesis of New Coumarin Derivatives

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In the 21st century, innovation has focused on green chemistry, environmental protection, and emerging diseases caused by new mutations. Cancer remains one of the deadliest illnesses, with no fully understood mechanism or universally effective treatment [1].

Modern medicine offers treatments like chemotherapy, hormonotherapy and radiation therapy, with chemotherapy being the most cost-effective and widely used. However, patients often require additional medications to manage side effects. New anti-cancer drugs, such as cisplatin and its derivatives, are highly effective but can cause side effects during treatment. To mitigate these effects, researchers are developing synthesis methods that attach chemotherapeutic drugs to biologically active ligands, reducing adverse reactions [2].

Coumarin-compounds can be the answer to this problem. They are the ones that are capable of avoiding the majority of side effects. Basic coumarin derivatives with minimal functional groups can be synthesized through simple chemical methods. However, producing coumarin derivatives with specific functional groups is less efficient, as reactions with the coumarin backbone have low yields and high synthesis costs. Our research's aim was the creation of a universal synthesis route for coumarin derivatives [3].

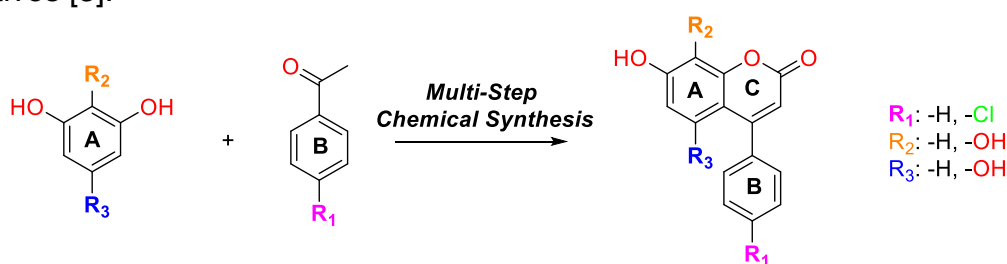


Figure 1: The possible synthetic route of the coumarin derivatives synthesis

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## **P11 1,3,4-Oxadiazole core as Building Block for Fluorescent Materials Design**

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In the quest for future's materials, hydrogels research area has witnessed an extraordinary turn over the last decade. Evolving from classical 3D cross-linked structures, modern hydrogels are currently carefully designed to integrate tailored functionalities in order to achieve desired properties. Notably, fluorescent hydrogels have gained significant attention due to their various applications in biosensing, data encryption and bioimaging [1]. However, their potential for versatile applications remains largely untapped due to limited tunability of their color emission [1].

One of the most interesting fluorescent structural motifs is represented by 1,3,4-oxadiazoles. They have high photoluminescence quantum yields, good chemical and thermal stability, and strong fluorosolvatochromism. Over time, numerous conjugated systems incorporating oxadiazole as the acceptor unit have been developed in order to modulate fluorescence emission. Due to high energy gap between HOMO and LUMO, these systems are well known for their emission in deep blue region [2]. Moreover, by regulating ICT processes, like ESIPT, emission can be shifted towards the green or yellow region [3], whereas by extending the system conjugation by introducing additional donor and acceptor units enables emission at lower frequencies, reaching the red domain [4], ultimately, covering the entire visible spectrum.

To use of oxadiazoles as fluorescent motifs in hydrogels systems remains unexplored because of several challenges including water insolubility, poor processability, and aggregation induced quenching effects at high oxadiazole content.

Herein, we report the synthesis and structural characterization of 1,3,4-oxadiazole congeners of well-established fluorescent motifs, the post-functionalization of poly(vinyl alcohol) with previously synthesized building blocks and the corresponding hydrogels synthesis. Their potential application in display technology or imaging is also pursued.

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## **P12 Assessment of the Antifungal Activity of Grape Pomace Extracts**

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The objective of this study was to evaluate the antifungal activity of extracts obtained from four varieties of grape pomace: two white varieties, Fetească Albă (FA) and Tămâioasă Românească (TR), and two red varieties, Fetească Neagră (FN) and Negru de Drăgășani (ND). This investigation was correlated with their phytochemical profiles, including total polyphenol content, total flavonoid content, and antioxidant activity. Based on the determined correlations (antifungal activity/phenolic compounds), the hypothesis that the grape pomace extracts can be used for viticulture as an alternative to synthetic fungicides was highlighted. The research aimed at (i) isolating some fungal species from natural environments, (ii) testing the antimicrobial activity of the extracts, and optimizing the nature of the extractant/extract concentration, (iii) obtaining the highest possible antifungal activity and, as far as possible, with a broad spectrum of action. The obtained grape pomace extracts demonstrated a variable activity of inhibiting the growth of the two tested fungal species, i.e., *Aspergillus* sp. and *Alternaria* sp. Pomace extracts (FA, TR, FN, ND) were shown to have superior antimicrobial activity against *Aspergillus niger* due to their higher concentration of polyphenols. FN and ND extracts did not exhibit antifungal activity against *Alternaria* sp., although the growth inhibition efficiency was lower compared to the growth inhibition of *Aspergillus* sp. The high concentration of bioactive compounds and the antioxidant capacity of the ND extract may be responsible for the antifungal activity exhibited by it. The results of the study can thus be used to develop new applications of extracts obtained from grapes, contributing to sustainable wine production, the protection of human health, and, last but not least, the environment.

## **P13 The Prediction Performance of Statistical Models and Neural Networks in a Microgrid Based on Energy Consumption from Renewable Sources**

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The main technologies used for residential purposes are power generation systems and solutions to reduce consumption, respectively, the implementation of smart management systems that could schedule the operation of the smart grid appliances by switching off the appliance for an energy saving condition when not in use [1]. The challenge that power providers face at peak times is optimizing power consumption from smart grids. These considerations have a considerable impact on the power system's reliability [2].

This research aims to forecast energy consumption from photovoltaic (PV) sources by implementing and comparing three different predictive models to improve interpretability, accuracy, and computational efficiency. The models selected in this approach are: ARIMA (Auto Regressive Integrated Moving Average), a statistical model for linear dependencies and trends; SARIMA (Seasonal ARIMA), an extension of ARIMA for seasonal fluctuations; and NAR (Nonlinear Auto Regressive Neural Network), a machine learning model for nonlinear relationships. The performance of these techniques is tested and confirmed using a dataset of real measurements related to the energy from photovoltaic sources' consumption, monitored at 15-minute intervals in 2024. The added value of the proposed approach consists of proving how improved forecasting directly contributes to energy efficiency and loss reduction in PV systems by enabling better energy management and demand-response strategies. This comparative analysis set up a solid foundation for the continued development of advanced forecasting models in energy systems. The findings emphasize the necessity of ongoing innovation in predictive analytics to support sustainable energy management and smart grid optimization.

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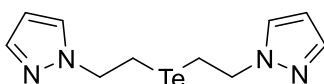
## **P14 Synthesis, Structure and Reactivity of a New Pyrazole-Containing Homoleptic Diorganotellurium(II) Compound**

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Interest in heavy organochalcogen compounds, such as selenium (Se) and tellurium (Te) derivatives, has surged in recent years due to their significant applications across various fields. In biology and medicine, they serve primarily as synthetic models for glutathione peroxidase [1]. In materials science, they are used as precursors for semiconducting materials **Error! Reference source not found.** Additionally, in organic synthesis, they function as catalysts or reagents in various organic transformations **Error! Reference source not found.** In contrast to organoselenium compounds, the organotellurium compounds, which share similar chemical characteristics with selenium, have been investigated to a much lesser extent. However, they also exhibit significant antioxidant activity.

Here we report the synthesis of a homoleptic diorganotellurium(II) ligand containing pyrazole groups (*Figure 1*). The obtained diorganotellurium(II) ligand was further reacted with silver, palladium and platinum salts. The new compounds were structurally characterized in solution by multinuclear NMR spectroscopy and mass spectrometry. The ionic structure of the palladium complex was determined by single crystal X-ray diffraction.



*Figure 1: The structure of the homoleptic diorganotellurium (II) ligand.*

*Acknowledgements:* This work was supported by UEFISCDI (Project PN-IV-P1-PCE-2023-0966).

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## **P15 Biocomposite Materials Based on Sawdust Biomass and Natural Polymers: Synthesis, Characterization and Potential for Biosorption Applications**

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Sawdust is a significant waste product of wood processing, ranging from logging activities to furniture fabrication. This type of waste, when stored in unregulated conditions, can readily contribute significantly to environmental pollution [1]. Water pollution, on the other hand, has emerged as a global concern, owing to the importance of water for consumption to all living species. First and foremost, emerging pollutants including pesticides, organic dyes, pharmaceutical chemicals, and more, are a serious threat to human health [2]. This study presents a simple and effective eco-friendly approach to valuing sawdust in environmental applications as adsorbent biomaterials. In this study, biocomposite materials were developed by immobilizing sawdust biomass in two natural polymers: alginate and chitosan. The obtained beads were evaluated for their ability to remove dyes and pharmaceuticals from aqueous matrices. The compounds chosen as target molecules were: ethacridine lactate (pharmaceutical compound); malachite green and brilliant green (organic dyes). Scanning electron microscopy (SEM) and Fourier-transform infrared spectroscopy (FTIR) were used to characterize the synthesized biosorbents. The size of the beads and the point of zero charge were also determined. In a batch system, lab-scale biosorption studies were carried out. Biosorbent sawdust/calcium alginate beads (SD-P1S6-A-5%) exhibited a spherical form, a diameter of  $3.0760 \pm 0.0700$  mm, a point of zero charge of 6.5, and textural stability when stored in calcium chloride solution at 4°C. The beads (SD-P1S6-C-2.5%) that were obtained using sawdust and chitosan showed an irregular form, measuring  $3.2060 \pm 0.0583$  mm in particle size and having a point of zero charge of 7.3. The results obtained for the two materials synthesized under the selected test conditions revealed a high removal efficiency. The biocomposite SD-P1S6-A-5% had a removal efficiency of 79.82% for the pharmaceutical compound and over 86% for the two dyes, whereas SD-P1S6-C-2.5% had a removal efficiency of more than 80% for all molecules examined. Sawdust-based biocomposite materials were discovered to be a potential biosorbent due to their high biosorption capability, low cost, and environmental friendliness.

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**P16 Synthesis and Characterization of Novel Azastibocine Halides**Tudor M. Ungurean<sup>1</sup>, Yann Sarazin<sup>2</sup>, Cristian Silvestru<sup>1</sup><sup>1</sup>*Supramolecular Organic and Organometallic Chemistry Centre, Faculty of Chemistry and Chemical Engineering, Babeş-Bolyai University, 11 Arany Janos Street, RO-400028, Cluj-Napoca, Romania*<sup>2</sup>*Institut des Sciences Chimiques de Rennes - ISCR UMR CNRS 6226, University of Rennes - Campus Beaulieu, 263 Av. Général Leclerc, 35042 Rennes, France  
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Organoantimony(III) halides are essential precursors in antimony chemistry. We synthesized two series of organoantimony(III) halides featuring two CNC-pincer ligands:  $[(CH_3)_2CHN(CH_2C_6H_4)_2]$  (series **a**) and  $[CH_3OCH_2CH_2N(CH_2C_6H_4)_2]$  (series **b**). The organolithium compounds **2a** and **2b** were obtained from the amines **1a** and **2b** via halogen-metal exchange using an improved method over previous literature [1,2]. The azastibocine chlorides were then synthesized via transmetalation with antimony trichloride. Heavier halides were obtained through halogen exchange with the corresponding chloride salts [1]. The methods used for **3b** [2] and **4a** [3] were improved compared to the previously reported ones by simplifying the workup. The synthesized organoantimony(III) halides exhibited air and moisture stability. All compounds were characterized by  $^1H$  and  $^{13}C\{^1H\}$  NMR spectroscopy, and the organolithium derivatives further analysed by  $^7Li\{^1H\}$  NMR spectroscopy. The solid-state structures of the **3a**, **5a**, **4a**, **4b** and **5b** were determined using single-crystal X-ray diffraction.

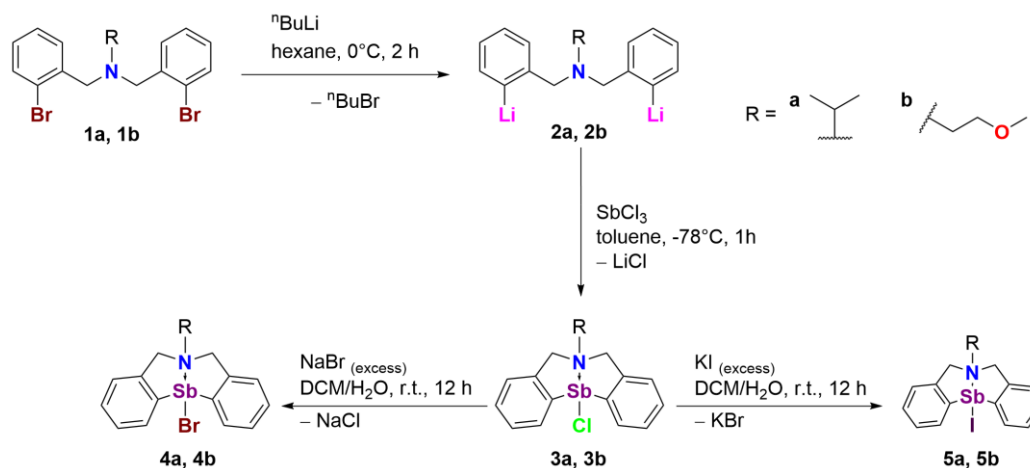


Figure 1: General synthetic pathway for obtaining azastibocine halides.

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## **P17 Pesticide and Heavy Metals Residues in Citrus Fruits: Human Exposure and Risks**

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**Abstract.** Numerous studies have shown that cumulative exposure to pesticide residues and/or heavy metals has far more harmful effects on human health than any single exposure. Statistically speaking, the number of food alerts caused by the presence of pesticide residues in fruit sold in the period 2017-2021 showed a spectacularly increasing number on the Romanian market and was correlated with the growing volume of imports and intra-EU trade during that period. This study aims to investigate the levels of pesticide residues and heavy metals, in citrus fruits (i.e. lemon, tangerine, orange, grapefruit, and lime) imported from non-EU and EU countries, in terms of human exposure and risks. In this regard, 69 samples were collected in the spring of the year 2024. Two European standards (i.e., EN 15662:2008 for determining pesticide residues and EN 15763:2009 for determining trace elements) were used in analytical investigations. The amount of pesticide residues in citrus samples was determined by gas chromatography-tandem mass spectrometry (GC-MS/MS). According to the GC-MS/MS results, out of 69 citrus samples, 41 samples had pesticide residues ranging from 0.005 to 2.700 mg/kg, and many samples had more active ingredients (like *o*-phenylphenol and spirodiclofen). The pesticide residue determination rate was 79 %. The results showed that the most identified pesticides in studied samples were imazalil, thiabendazole, pyrimethanil, pyraclostrobin, fludioxonil, spirodiclofen, and *o*-phenylphenol. In addition, 17 citrus peel extract samples were analyzed to determine concentrations of several metals, including Al, Cr, Mn, Ni, Cu, Zn, Sr, Cd, and Pb, by inductively coupled plasma mass spectrometry technique (ICP-MS). Analytical data showed that in all analyzed citrus samples, the concentration of Cd and Pb, in terms of carcinogenic and potentially carcinogenic metals respectively, did not exceed the MRLs set according to Regulation 2023/915/EC. The findings of the statistical analysis indicate a positive correlation between Cu and Zn. The relationships between Al and Sr, Cr and Ni, Cr and Zn, Cr and Pb, Mn and Zn, Ni and Cd, Ni and Pb, Cd, and Pb are also positively correlated (>0.500). This study, for the first time, assessed the health risks of oral exposure to a mixture of pesticides and metals through the consumption of different *Citrus* fruits for Romanian consumers.

**Keywords:** fruit Citrus, pesticide, heavy metals, GC-MS/MS, ICP-MS, statistical analysis, health risk.

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